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THE BOUNDARY ELEMENT METHOD APPLIED TO THE TWO DIMENSIONAL STEFAN MOVING BOUNDARY PROBLEM

THESIS

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This thesis considers problems for which the boundary is not known before the problem is solved and must be determined as part of the solution. We consider a time dependent problem which results in a moving boundary. We look at the heat conduction/diffusion equation in one and two spatial dimensions. We use Green's Theorem to yield a Volterra boundary integral equation which involves an unknown function on the moving boundary. We use the boundary element method to obtain a solution. Graphical results for the two dimensional problem are presented.

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THESIS

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of the Air Force Institute of Technology
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Master of Science (Computer Systems)

Donald C. Vosika, B.S.,B.S.E.E.
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I would like to thank my parents for all that they have taught me. The common sense that I acquired in growing up on a farm with them has proven invaluable.

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There are no words that can describe my debt to my wife, Cheryl. Without her help and inspiration, this thesis would not exist. She was always there when I needed her most. I am so very fortunate to be able to share the sun, the sand, and the warm sea with her.

And now there will be time for the southern sunsets, the tropical seas, and the beautiful fishes ...

Donald C. Vosika

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Abstract

In this thesis we consider problems for which the boundary is not known before the problem is solved and must be determined as part of the solution. We consider a time dependent problem which results in a moving boundary. We look at the heat conduction/diffusion equation in one and two spatial dimensions. We introduce the fundamental solution or Green's function and use Green's Theorem to yield a Volterra boundary integral equation which involves an unknown function on the moving boundary. We take the limit of our integral expression to the moving boundary to obtain a nonlinear system of integral equations for the location of the boundary and the unknown function. We use the boundary element method to obtain a solution to this system of integral equations. This solution is then substituted back into the original Volterra equation to obtain the solution of our original problem. Graphical results for the two dimensional problem are presented.

THE BOUNDARY ELEMENT METHOD APPLIED TO THE TWO DIMENSIONAL STEFAN MOVING BOUNDARY PROBLEM

I. Introduction

1.1 Backround

Typically, the goal in solving differential equations is to find a solution of the equation on some domain Ω given the value of the solution or the value of the normal derivative of the solution on the boundary Γ of the domain. But, there is a class of boundary value problems for which the boundary is not known in advance and must be determined as part of the solution. These problems are known as unknown boundary problems. If the differential equation is steady state (no time derivatives) then the boundary will be unknown but will remain fixed. These are known as free boundary problems. If the equation is evolutionary then the boundary will move as a function of time and the domain on which we are solving the differential equation will be time-dependent. These are known as moving boundary problems. This thesis will deal with a two-dimensional moving boundary problem. In order to solve a problem with an unknown boundary, we must impose extra conditions on the solution's behavior at the boundary in addition to the typical boundary and initial conditions. These extra conditions are often drawn from physical concerns such as the conservation of energy or the physical spatial constraints imposed on a real-world problem.

Unknown boundary problems arise frequently in the physical world. They can be found in the study of the solidification of metals, carbon diffusion in steelmaking,

ablation of materials using a laser beam, welding of two metals, corrosion and oxidation of metals, oxygen diffusion in biological tissues, the melting and freezing of ice, thermal switching of glasses, stellar evolution, diffusive chemical reactions, electrochemical machining, water seepage through dams, impulse and optimal control, and crystal growth. This thesis will look at an example involving the melting and freezing of ice.

When considering the melting of ice it is possible to have a single phase problem or a two phase problem. In the single phase, the ice is initially at it's melting temperature $U = 0°C$ and only the heat of fusion need be transferred in order to melt it. In the two phase problem, the ice is initially at some temperature below it's melting point and we must transfer heat energy in order to bring it to the melting point and then supply additional heat energy in order to satisfy the heat of fusion. We will consider the single phase problem in this thesis.

1.2 Goals

The goals of this thesis are:

1. To model phase change problems in one and two dimensions.
2. To apply the boundary element technique to a two dimensional melting ice problem.
3. To use computer graphics as a tool to display the numerical results in a visual format.

1.3 Scope

We have limited ourselves to two dimensions and to a circular initial domain in order to have an analytic solution available for comparison with the numerical calculation results. Isotropic materials are considered to simplify the heat energy exchange. Relatively short time intervals are considered to avoid excessive calculation time. Grid refinement is kept as minimal as possible. also to avoid excessive computation time. We neglect changes in the density under phase transitions in

order to avoid dealing with convection currents. Convection currents will occur if the density is allowed to change even if the liquid phase is incompressible and its thermal expansion can be neglected (3:227). It should be noted that our model can be directly applied to diffusion problems.

1.4 Support

We required the use of a number of computer systems and software packages in order to complete this thesis. The main thrust of the computation was borne by the AFIT ELXSI computer. The large number of test runs and the length of the runs made the use of this computer a necessity. Shorter length computations were performed on a VaxStation II/GPX belonging to WL/AARM. Text processing was borne by AFIT's Scientific Support Computer VAX 11/785 and also by a WL/AARM VAX 11/785. The text processing was accomplished with the LaTeX Document Preparation System.

The programming code was written in the Fortran programming language. This language was chosen because it is a standard programming language for which optimized compilers are readily available. All of the code is compliant with the ANSI X-3.9 1978 (Fortran-77) standard. The support command language routines were written in the Csh shell programming language. Various Unix utilities, such as awk and sort, were used in the shell scripts.

The graphics output was generated by subroutine calls to the metalib graphics package on the Scientific Support Computer and by the CA-DISSPLA graphics package on the WL VAXen. The metalib software is a local adaptation of a package that was developed at the Air Force Weapons Laboratory at Kirtland AFB. Local enhancements were made by Lt Col James Lupo of AFIT/ENP. The AFIT Sun workstation network was utilized in running the Mathematica software for calculations involving Bessel functions.

1.5 *Mathematical History of the Problem*

Moving boundary problems are often referred to as Stefan problems due to the work done by J. Stefan, in 1889, on the freezing of the ground (21:173–484) and the melting of ice layers (22:965–983).

Actually, the first work in the moving boundary area was performed by G. Lamé and B.P. Clapeyron in 1831. They tried to calculate the thickness of a solid crust on liquid cooling in the half space $x > 0$ with a constant temperature on the plane $x = 0$. They discovered that the thickness is proportional to the square root of time but did not arrive at the constant of proportionality (13:25—256).

There are few analytic solutions to moving boundary problems in closed form. Generally, they are for a one-dimensional geometry on an infinite or semi-infinite domain with simple boundary and initial conditions and having constant thermal properties. The solutions are usually functions of the single variable $x/\sqrt{t}$ and are called similarity solutions. Both of the problems that Stefan worked on possess similarity solutions of the form $u = 2\alpha\sqrt{t}$. The value of α can be determined from transcendental equations (17:2). The motive behind similarity solutions is to reduce the number of independent variables by taking an algebraic combination of them (1:63–75).

M. Brillouin reduced the solution of the Stefan problem to a system of nonlinear integro-differential equations in 1929 (2:285–308). However, he did not try to solve the system as he thought it would be very difficult to do so.

In 1931, L.S. Leǐbenzon derived an approximation for the solution of the Stefan problem for many cases (14:435–439). He replaced the true temperature distribution by a quasi-stationary solution. This solution obeyed the Laplace equation in space in a domain that had a moving boundary that corresponded with the solution of Stefan.

Another analytic solution technique used in moving boundary problems is transforming the coordinates so the moving boundary becomes fixed in the new coordinate system. The concept of conformal transformations is used in the hodograph method which finds frequent application in the field of fluid mechanics. The hodograph method is presented in (4:288–293) and (15).

Numerical methods applied to unknown boundary problems have an extensive repertoire. Since the solution of the unknown boundary problem requires that we solve the known boundary problem, the numerical techniques for known problems find use in the unknown domain. In addition to using the known techniques, we are able to change the unknown problem by transformations before their application if we so choose.

If we do not manipulate the unknown boundary problem, then we must explicitly approximate the boundary throughout our calculations. This approach is called the trial-free-boundary method for free boundary problems and is called the front-tracking method for moving boundary problems. We will discuss these methods later in this thesis.

If we do transform the problem before trying to solve it, then we temporarily remove the unknown boundary. This introduces some complications, however. The transformed problem will be nonlinear since the original unknown boundary problem was nonlinear. And we have to perform a recovery transform to get back the unknown boundary at the end of the calculations. The types of transformations we could use are called front-fixing, analytical, and fixed-domain.

In the front-fixing method, the unknown domain is transformed onto a known domain with a more complex differential equation and boundary conditions. An example of this method is the isotherm migration technique.

In the analytical method, we use techniques such as conformal mapping to obtain a new problem such as an integral equation. Helmholtz used conformal map-

ping to solve fluid flow free boundary problems in 1868. His work was extended by Kirchhoff in 1869 (5:614). In 1986, Elcrat and Trefethen made their techniques the basis of an efficient and effective method for solving integrals that are like those found in Schwarz-Christoffel mappings (6:251–265).

The fixed-domain method uses a weak or generalized solution defined on a known domain that implicitly has information about the unknown boundary. Examples of this method are variational inequalities and the enthalpy method for Stefan problems. Baiocchi used variational inequalities to study porous flow problems in earthen dams (5:618). The enthalpy H denotes the total heat content in a region. The enthalpy method can be applied to "mushy" regions that are the result of the mixture of two phases such as water and ice. This method is advocated by Solomon, Alexiades, and Wilson (20:8–12).

This thesis will solve a moving boundary problem in its original form. The trial-free-boundary method and the front-tracking method often need to be applied to domains with curved boundaries. The approaches which are the most popular use integral equations, finite-differences with boundary-fitted coordinates, or finite elements. The boundary element method we will apply will generate a Volterra integral equation which will allow us to integrate around the boundary of the domain instead of a double integral over the area of the domain and will thus simplify the calculations.

Rubinstein provided existence and uniqueness proofs for the one-dimensional Stefan problem with general initial conditions in 1947 (18:37–54). Originally, he transformed the domains for each phase to the interval $[0, 1]$ by reducing the problem to a system of nonlinear integral equations of mixed type (Fredholm with respect to space and Volterra with respect to time). This system could then be solved by Picard's method of successive approximation. However, it required the evaluation of double integrals and was therefore not effective. Again, in 1947, he gave a method of reducing the Stefan problem to integral equations of Volterra type based on direct

use of the heat potential (19:217–220). Existence and convergence was guaranteed in the small; i.e., in some neigborhood of $t = 0$.

Kolodner (12:1–31) used integral equations to solve the Stefan problem of the freezing of a finite depth lake in the 1950's. He incorporated simple Green's functions in his solution. He noted that the cases of physical interest generate Volterra integral equations of the second kind. These integral equations can be solved by numerical methods even though they possess difficulties near $t = 0$.

Avner Friedman carried out detailed research in the problems of the evaporation of a spherical drop (8:19–66) and the dissolution of a gas bubble in a liquid (9:327–345). He also showed the application of the maximum principle to the Stefan problem (10:201–211). Later, he compiled a text on parabolic partial differential equations including a separate chapter on the Stefan problem (7). He demonstrates how a parabolic differential equation can be transformed into a Volterra integral equation which can then be solved by the method successive approximations. This is the approach that will be used in this thesis. In addition, we will utilize the boundary element method in performing the integrations required for the solution of the Stefan problem.

Stefan problems are essentially nonlinear because of the condition on the moving boundary, but linearity usually exists in each of the domains on both sides of the boundary and we can still utilize the integral equation approach. It has the advantage that only the values of the unknowns on the boundary enter into the solution when it is coupled with the boundary element technique.

II. Mathematical Development

2.1 The Heat Equation

The partial differential equation which we are trying to solve is

$$c\rho\frac{\partial u}{\partial t} = \nabla \cdot (K_0 \nabla u) + Q$$

where c is the specific heat of the material, ρ is the mass density, u is the temperature, t is time, K_0 is the thermal conductivity, and Q is the heat energy generated within the domain of interest. If there are no sources or sinks within the domain then $Q = 0$. Also, if we assume a homogeneous isotropic material with constant thermal properties then the constants can be combined into a single constant $K = K_0/c\rho$. We arrive at the heat equation

$$\frac{\partial u}{\partial t} = K\nabla^2 u$$

For one dimension the heat equation becomes

$$\frac{\partial u}{\partial t} = K\frac{\partial^2 u}{\partial x^2}$$

And for two dimensions we have

$$\frac{\partial u}{\partial t} = K(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2})$$

In order to solve the heat equation on a domain, we must supply initial and boundary conditions.

2.2 Boundary Conditions

In solving differential equations it is not sufficient to state only the equation itself. A particular equation could have an infinite number of solutions. In order to

select a single unique solution out of this infinite number, it is necessary to specify initial and/or boundary conditions for the equation. Attempting to fit a solution to the conditions can be as difficult as trying to solve the differential equation in the first place.

Initial conditions are those that must be satisfied by the solution throughout the domain at the instant when consideration of the system begins. A typical initial condition will prescribe both the solution at the beginning time and the time derivatives up through order $m-1$ at the beginning time. Here m is the order of the highest time derivative in the differential equation.

Boundary conditions specify the value of the solution on the boundary of the domain (Dirichlet condition), the normal derivative of the solution on the boundary of the domain (Neumann condition), or a combination of value and normal derivative on the boundary (Robin or mixed condition).

The prescribed initial and boundary conditions, together with the coefficients and any inhomogeneous terms in the partial differential equation, comprise the "data" in the problem modeled. The solution depends continuously on the data if small changes in the data produce correspondingly small changes in the solution.

A problem that is modeled by the partial differential equation is said to be "well-posed" if:

1. A solution to the problem exists.
2. The solution is unique.
3. The solution depends continuously on the data.

If any of these conditions is not satisfied, then the problem is said to be "ill-posed."

Because the heat equation is evolutionary, it is necessary to specify an initial condition. However, it involves only the first time derivative of the temperature. Therefore, it will require specifying only the value of the solution at the initial time

value and not the values of any time derivatives. If we specify the value of the solution at any time other than the initial time, the problem may not be well-posed. This is related to the fact that it is difficult to solve the heat equation backwards in time. At any time $t > t_{initial}$, the solution to the initial value problem at an arbitrary point in the domain depends on "all" of the initial data. This implies an infinite speed of propagation of effects.

The specification of the initial condition along with the behavior of the solution at infinity constitutes a Cauchy problem for the heat equation. A solution to the Cauchy problem is infinitely differentiable with respect to position and time for each point in the domain and for all values of time greater than the initial instant. This shows the smoothing property of the heat evolution operator. A sectionally continuous initial state can always evolve forward in time. However, if it is not infinitely differentiable with respect to both position and time, then it cannot have originated from an earlier state. Thus, the heat equation is irreversible in that "forward" time is distinguishable from "backward" time. This property in the mathematical model corresponds with the second law of thermodynamics in the physical world modeled.

Thus we see that we must have the correct number of initial and boundary conditions of the correct type in order for our problem to be well-posed and to have a physically realizable solution.

2.3 The Method of Successive Approximations

In order to describe the method of successive approximations, we begin by considering the space $\mathcal{C}_b$ of bounded continuous functions. If $A \subset \mathbf{R}^n$, let $\mathcal{V}$ be the set of all functions $f : A \to \mathbf{R}^m$. The zero function is the member of $\mathcal{V}$ that maps each $x \in A$ to the zero element of $\mathbf{R}^m$. We define addition on $\mathcal{V}$ by $(f+g)(x) = f(x)+g(x)$ for all $x \in A$ and for all $f, g \in \mathcal{V}$. Also, we define multiplication by a scalar on $\mathcal{V}$ by $(\lambda f)(x) = \lambda(f(x))$ for each $\lambda \in \mathbf{R}$ and $f \in \mathcal{V}$. Then, $\mathcal{V}$ is a vector space. We now consider the subspace $\mathcal{C}$ of $\mathcal{V}$ defined by $\mathcal{C} = \{f \in \mathcal{V} \mid f \text{ is continuous}\}$.

The subspace $\mathcal{C}$ of continuous functions is also a vector space. We now choose the subspace $\mathcal{C}_b$ of $\mathcal{C}$ to be the elements of $\mathcal{C}$ that are bounded, i.e., $\mathcal{C}_b = \{f \in \mathcal{C} \mid \|f(x)\| < M \text{ for all } x \in A, M \text{ constant} \in \mathbf{R}\}$. If A is compact, then $\mathcal{C}_b = \mathcal{C}$ since continuous mappings on a compact set are bounded. The new space $\mathcal{C}_b$ is also a vector space. We define a norm on $\mathcal{C}_b$ by $\|f\| = \sup\{|f(x)| \mid x \in A\}$ for all $f \in \mathcal{C}_b$. This norm will exist since f is bounded. Every Cauchy sequence in $\mathcal{C}_b$ converges to a point in $\mathcal{C}_b$, so $\mathcal{C}_b$ is complete. Thus, $\mathcal{C}_b$ is a complete normed space which is equivalent to saying that it is a Banach space.

A contraction mapping is any map $T : \mathcal{C}_b(A, \mathbf{R}^m) \rightarrow \mathcal{C}_b(A, \mathbf{R}^m)$ such that $\exists$ a constant $\lambda \in \mathbf{R}$, $0 \leq \lambda < 1$ and $\|T(f) - T(g)\| \leq \lambda\|f - g\|$ for all $f, g \in \mathcal{C}_b(A, \mathbf{R}^m)$. The mapping T is continuous and there is a unique point in $\mathcal{C}_b$ that is mapped to itself, i.e., $\exists\ f_0 \in \mathcal{C}_b(A, \mathbf{R}^m)$ such that $T(f_0) = f_0$. The point f_0 is called a fixed point of the mapping. We now form the sequence

$$
\begin{aligned}
x_0 &= f \\
x_1 &= T(f) \\
x_2 &= T(T(f)) &&= T^2(f) \\
x_3 &= T(T(T(f))) &&= T^3(f) \\
&\vdots \quad \vdots && \quad \vdots
\end{aligned}
$$

This sequence is a Cauchy sequence and it converges to the unique fixed point of the mapping T. Thus, we see that if we have a system which is described by a contractive mapping or transformation that we are guaranteed to converge to a unique solution if we take the output from the system and apply it again to the input in a repetitive feedback process. This process is illustrated in Figure (2.1). This is the essence of the method of successive approximations. We determine an initial "guess" for the solution to our contractive system. We then input this initial solution into the system to obtain a new solution. This new solution is then used as input to the system and this process is repeated until we have achieved the required convergence.

We can illustrate the method by applying it to the solution of an integral equation. Consider the equation

$$f(x) = a + \int_0^x k(x, \xi) f(\xi) d\xi \tag{2.1}$$

This equation is a transformation on the function f since we can write it as

$$T(f)(x) = a + \int_0^x k(x, \xi) f(\xi) d\xi$$

The transformation T will be contractive and there will be a unique solution on the interval $[0, r]$ if

$$\sup_{x \in [0,r]} \int_0^x |k(x, \xi)| d\xi = \lambda < 1$$

This places a restriction on the kernel of the integral equation transformation $k(x, \xi)$. The solution will be the function $f(x)$ that is the fixed point of the transformation. We solve equation (2.1) with an appropriate kernel by making a trial guess for $f(\xi)$ and substituting it into the right hand side of the equation. We perform the operations required by the equation and obtain a new function $f(x)$ on the left hand side of equation (2.1). This new function can then be substituted back in the right hand side and the process repeated. As the process is repeated, we compare the new function created with the old function that was input. When they are as close as we require, the repetitive cycle is stopped and we have converged to our solution $f(x)$. We will show later how to apply this method to the solution of the Stefan problem in one and two dimensions.

2.4 The One Dimensional Problem

Our first example is one dimensional diffusion or heat propagation. The problem considered in this section is consistent with the problem presented in (7:216) where existence and uniqueness results are presented. Suppose U satisfies

$$
\begin{aligned}
U_t &= U_{xx} && 0 < x < s(t),\ \ t > 0 \\
U(0,t) &= f(t) && f(t) \geq 0,\ \ t > 0 \\
U(x,0) &= \phi(x) && \phi(x) \geq 0,\ 0 < x \leq b, \\
& && \phi(b) = 0,\ b > 0 \\
U(s(t),t) &= 0 && t > 0,\ s(0) = b \\
U_x(s(t),t) &= -\frac{1}{k}\frac{d}{dt}s(t) && t > 0
\end{aligned}
$$

The boundary condition for the end $x = 0$ is non-homogeneous. The boundary condition on the moving boundary, $x = s(t)$, is homogeneous (Dirichlet). The initial condition is non-homogeneous. We know from physical constraints that the temperature in the domain must be bounded. This set of conditions along with the partial differential equation form a well-posed problem. The domain of interest for this problem is shown in Figure (2.2). To solve this problem, we use Green's Theorem as follows. We suppose that U satisfies the equation

$$U_\tau = U_{\xi\xi}$$

and, following (7:220), choose

$$G(x,t;\xi,\tau) = K(x,t;\xi,\tau) - K(-x,t,\xi,\tau)$$

where

$$K(x,t;\xi,\tau) = \frac{1}{2\pi^{1/2}(t-\tau)^{1/2}} \exp\left[-\frac{(x-\xi)^2}{4(t-\tau)}\right]$$

so $G(x,t;\xi,\tau)$ satisfies the adjoint equation

$$G_\tau = -G_{\xi\xi}$$

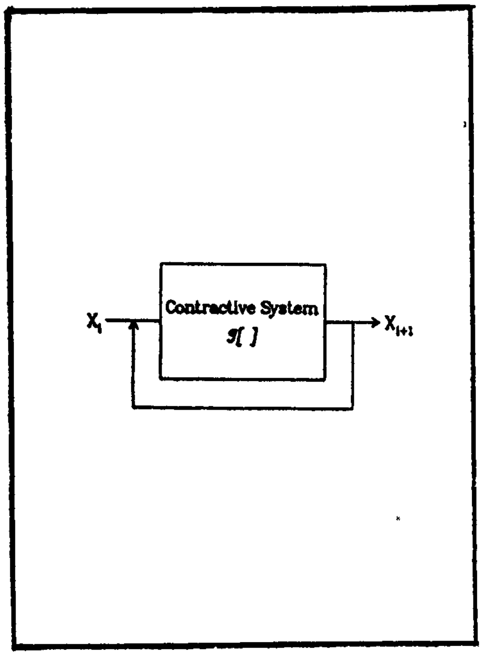


Figure 2.1. Feedback in a Contractive System

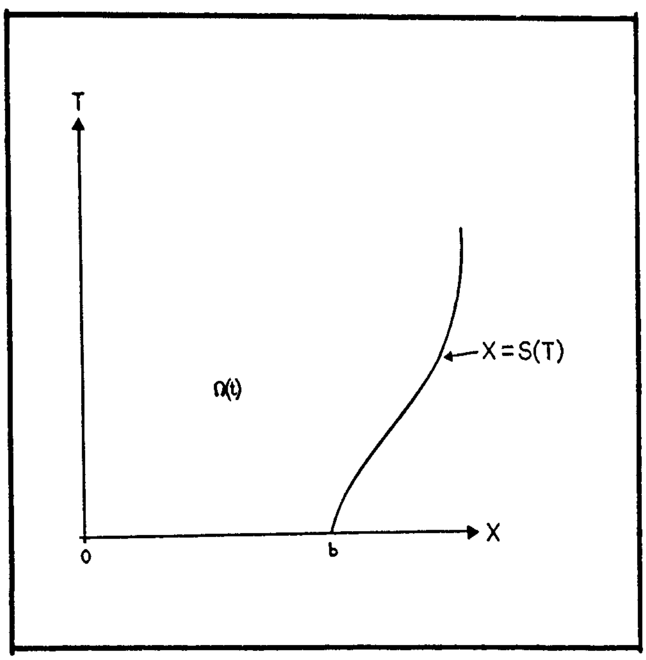


Figure 2.2. Domain for the One Dimensional Problem

with the boundary condition at $\xi = 0$

$$G(x, t; 0, \tau) = 0$$

Then, we introduce Green's identity

$$0 = (GU_\xi - UG_\xi)_\xi - (GU)_\tau \tag{2.2}$$

and we integrate equation (2.2) with respect to ξ from 0 to $s(\tau)$ and with respect to τ from 0 to $t - \epsilon$ to obtain

$$\begin{aligned}
0 &= \int_0^{t-\epsilon} \int_0^{s(\tau)} [(GU_\xi - UG_\xi)_\xi - (GU)_\tau] d\xi d\tau \\
&= \int_0^{t-\epsilon} \int_0^{s(\tau)} (GU_\xi - UG_\xi)_\xi \, d\xi d\tau \\
&\quad - \int_0^{t-\epsilon} \int_0^{b} (GU)_\tau d\xi d\tau \\
&\quad - \int_0^{t-\epsilon} \int_b^{s(\tau)} (GU)_\tau d\xi d\tau \\
&= \int_0^{t-\epsilon} (GU_\xi - UG_\xi) \,|_{\xi = s(\tau)} d\tau \\
&\quad - \int_0^{t-\epsilon} (GU_\xi - UG_\xi) \,|_{\xi=0} d\tau \\
&\quad - \int_0^{b} \int_0^{t-\epsilon} (GU)_\tau d\tau d\xi \\
&\quad - \int_b^{s(t-\epsilon)} \int_{s^{-1}(\xi)}^{t-\epsilon} (GU)_\tau \, d\tau d\xi
\end{aligned} \tag{2.3}$$

In equation (2.3) we have used the fact that for any integrable function $F(\xi, \tau)$.

$$\begin{aligned}
\int_0^{t-\epsilon} \int_0^{s(\tau)} F(\xi, \tau) d\xi d\tau &= \int_0^{t-\epsilon} \int_0^{b} F(\xi, \tau) d\xi d\tau \\
&\quad + \int_0^{t-\epsilon} \int_b^{s(\tau)} F(\xi, \tau) d\xi d\tau
\end{aligned}$$

and have interchanged the order of integration in the last two integrals in (2.3). We are guaranteed that we can change the order of integration by Fubini's Theorem which states:

$$\int \left\{ \int F(\xi,\tau) d\xi \right\} d\tau = \int \left\{ \int F(\xi,\tau) d\tau \right\} d\xi$$

This relation holds for Lebesgue integrals whenever

$$\int \int |F(\xi,\tau)|\, d\xi d\tau < \infty$$

Fubini's Theorem applies to Riemann integrals when they exist. If we take into account that $U(s(\tau),\tau) = 0$ and that $G(x,t;0,\tau) = 0$, equation (2.3) becomes

$$\begin{aligned}
0 \;=\; & \int_0^{t-\epsilon} G(x,t;s(\tau),\tau) U_\xi(s(\tau),\tau) d\tau \\
& + \int_0^{t-\epsilon} G_\xi(x,t;0,\tau) f(\tau) d\tau \\
& - \int_0^{b} G(x,t;\xi,t-\epsilon) U(\xi,t-\epsilon) d\xi \\
& + \int_0^{b} G(x,t;\xi,0) U(\xi,0) d\xi \\
& - \int_b^{s(t-\epsilon)} G(x,t;\xi,t-\epsilon) U(\xi,t-\epsilon) d\xi \\
& + \int_b^{s(t-\epsilon)} G(x,t;\xi,s^{-1}(\xi)) U(\xi,s^{-1}(\xi)) d\xi
\end{aligned} \tag{2.4}$$

Combining the third and fifth integrals, taking into account that $U(\xi,s^{-1}(\xi))|_{\xi>b} = 0$, and taking the limit as $\epsilon \to 0$ we obtain

$$\begin{aligned}
U(x,t) \;=\; & \int_0^{t} G(x,t;s(\tau),\tau) U_\xi(s(\tau),\tau) d\tau \\
& + \int_0^{t} G_\xi(x,t,0,\tau) f(\tau) d\tau \\
& + \int_0^{b} G(x,t;\xi,0) U(\xi,0) d\xi
\end{aligned} \tag{2.5}$$

If we take $\frac{\partial}{\partial x}$ of both sides of equation (2.5) and take the limit as $x \to s(t)$ and let $V(x,t)|_{x=s(t)} = \frac{\partial}{\partial x} U(x,t)\Big|_{x=s(t)}$ we obtain

$$\begin{aligned} V(x,t)|_{x=s(t)} &= \frac{1}{2} V(x,t)|_{x=s(t)} + \int_0^t G_x(s(t),t;s(\tau),\tau)V(s(\tau),\tau)d\tau \\ &+ \int_0^t G_{x\xi}(s(t),t;0,\tau)f(\tau)d\tau \qquad (2.6) \\ &+ \int_0^b G_x(s(t),t;\xi.0)\phi(\xi)d\xi \end{aligned}$$

(2.7)

For details concerning the limit we have taken see Appendix B. We now integrate the boundary condition

$$U_x(s(t),t) = -\frac{1}{k}\frac{d}{dt}s(t) \quad t > 0$$

from $\tau = 0$ to $\tau = t$ to obtain

$$s(t) = b - k\int_0^t V(s(\tau),\tau)d\tau \qquad (2.8)$$

where we have used the facts that $s(0) = b$, k is a constant independent of t, and $V(x,t)|_{x=s(t)} = \frac{\partial}{\partial x} U(x,t)\Big|_{x=s(t)}$.

We use equations (2.6) and (2.8) as the key part of the solution algorithm for the one dimensional Stefan problem.

Algorithm 1:

1. Guess $s_0(t)$, $V_0(x,t)|_{x=s(t)}$.
2. Substitute into the right hand side of (2.6) and (2.8) to obtain $s_1(t)$, $V_1(x,t)|_{x=s(t)}$ from the left hand side of (2.6) and (2.8).
3. Iterate until convergence.
4. Substitute $s_n(t)$ and $V_n(t)$ into (2.5) to obtain $U(x,t)$.

This algorithm is the embodiment of the method of successive approximations. In step (1), we generate the initial input for the method. In step (2), we apply the input to the system in order to allow the contractive transformations to give us a "better" estimate of the solution to the system. We then apply this better estimate to the system input in a feedback iteration loop in step (3). We repeat until the output from the system is within the accuracy envelope of the input that we have determined we require. We are guaranteed that we will obtain convergence since the transformations are contractive. We then use the solutions we obtained for the moving boundary position $s(t)$ and the heat flux $V(t)$ by the method of successive approximations in the equation for the temperature $U(x,t)$ in step (4).

2.5 *The Two Dimensional Problem*

We now consider the two dimensional problem. Suppose that U satisfies

$$\begin{aligned}
U_t &= a^2(U_{xx}+U_{yy}) && (x,y)\in\Omega(t),\quad 0<t<T \\
U(x,y,t) &= 0 && (x,y)\in\Gamma(t)=\partial\Omega(t) \\
U(x,y,0) &= \phi(x,y) && (x,y)\in\Omega(0) \qquad (2.9)\\
\frac{dx}{dt} &= -k_1U_x(x,y,t) && (x,y)\in\Gamma(t) \\
\frac{dy}{dt} &= -k_2U_y(x,y,t) && (x,y)\in\Gamma(t)
\end{aligned}$$

We see that we have a homogeneous (Dirichlet) boundary condition for the temperature on the boundary. The initial condition is non-homogeneous. Again, we know from physical constraints that the temperature in the domain must be bounded. We also require that the temperature be bounded at the origin $x = y = 0$. This will lead to our expressing the theoretical solution to the fixed boundary problem in terms of a Bessel function of the first kind of order zero. We will give details on this solution in the next chapter. This set of conditions along with the partial differential equation are a well-posed problem. The domain of interest for this problem is shown in Figure (2.3). The velocity of the moving boundary is proportional to the energy flow across the boundary since the melting of the ice is directly proportional to the amount of heat energy transferred. Fourier's law states that the heat flux is proportional to the temperature gradient:

$$\vec{\Phi} = -k\nabla U \tag{2.10}$$

The minus sign is due to the fact that heat energy flows in the direction of decreasing temperature so that the heat flow vector is in the opposite direction to the temperature gradient. Therefore, the velocity of the moving boundary is proportional to the temperature gradient:

$$\begin{aligned} \vec{v} &= -k_0\nabla U \\ &= -k_0(\vec{\imath}U_x + \vec{\jmath}U_y) \end{aligned} \tag{2.11}$$

Since

$$\vec{v} = \vec{\imath}\frac{dx}{dt} + \vec{\jmath}\frac{dy}{dt} \tag{2.12}$$

we have:

$$
\begin{aligned}
\frac{dx}{dt} &= -k_0 U_x \\
\frac{dy}{dt} &= -k_0 U_y
\end{aligned}
\tag{2.13}
$$

To allow for different expansion rates in the $\vec{\imath}$ and $\vec{\jmath}$ directions we assume different proportionality constants k_1 and k_2 and arrive at the last two equations in (2.9). Thus these equations represent the transfer of latent heat necessary to melt or freeze the ice. They are known as 'Stefan conditions'. These expressions for dx/dt and dy/dt are similar to expressions found in (16:741–752). Since the heat operator $L = \partial/\partial t - a^2\nabla^2$ is not self-adjoint, we introduce the adjoint operator $L^* = -\partial/\partial t - a^2\nabla^2$ and obtain the adjoint equation:

$$
G_\tau + a^2(G_{\xi\xi} + G_{\eta\eta}) = 0 \tag{2.14}
$$

If U satisfies (2.9) and G satisfies (2.14) then

$$
0 = a^2[(U_\xi G)_\xi + (U_\eta G)_\eta - (UG_\xi)_\xi - (UG_\eta)_\eta] - (UG)_\tau
$$

If we integrate this equation with respect to τ from 0 to $t - \epsilon$ and with respect to ξ and η on the region $\Omega(\tau)$ and let $\hat{\Omega}(\tau) = \Omega(\tau) - \Omega(0)$, we obtain

$$
\begin{aligned}
0 &= \int_0^{t-\epsilon}\int_{\Omega(\tau)} \{[a^2\, U_\xi\, G]_\xi + [a^2\, U_\eta G]_\eta\} d\xi d\eta d\tau \\
&- \int_0^{t-\epsilon}\int_{\Omega(\tau)} \{[a^2\, UG_\xi]_\xi + [a^2 UG_\eta]_\eta + (UG)_\tau\} d\xi d\eta d\tau \\
&= \int_0^{t-\epsilon}\int_{\Gamma(\tau)} [a^2 U_\xi G \hat{n}_\xi + a^2 U_\eta G \hat{n}_\eta] d\sigma d\tau \\
&- \int_0^{t-\epsilon}\int_{\Gamma(\tau)} [a^2 UG_\xi \hat{n}_\xi + a^2 UG_\eta)\hat{n}_\eta] d\sigma d\tau \\
&- \int_0^{t-\epsilon}\int_{\Omega(0)} (UG)_\tau d\xi d\eta d\tau - \int_0^{t-\epsilon}\int_{\hat{\Omega}(\tau)} (UG)_\tau d\xi d\eta d\tau
\end{aligned}
\tag{2.15}
$$

In equation (2.15) we have used Green's Theorem $\oint_C \vec{A} \cdot \hat{n}\ ds = \int_R \int \nabla \cdot \vec{A}\ dxdy$ to obtain the boundary integrals on $\Gamma(\tau)$ from the area integrals over $\Omega(\tau)$. For $(\xi, \eta) \in \hat{\Omega}(t-\epsilon)$, let $t^*(\xi, \eta)$ be determined by $(\xi, \eta) \in \Gamma(t^*)$.

We can now interchange the order of integration in the last two integrals in equation (2.15) and take these two integrals to the left hand side of the equation to obtain

$$\int_{\Omega(0)} \int_0^{t-\epsilon} (UG)_\tau d\tau d\xi d\eta + \int_{\hat{\Omega}(t-\epsilon)} \int_{t^*(\xi,\eta)}^{t-\epsilon} (UG)_\tau d\tau d\xi d\eta$$
$$= \int_0^{t-\epsilon} \int_{\Gamma(\tau)} \left(a^2 G \frac{\partial U}{\partial n} - a^2 U \frac{\partial G}{\partial n} \right) d\sigma\ d\tau \qquad (2.16)$$

In equation (2.16), we have used $\partial U / \partial n = U_\xi \hat{n}_\xi + U_\eta \hat{n}_\eta$. Thus

$$\int_{\Omega(0)} [UG|_{\tau=t-\epsilon} - UG|_{\tau=0}]\, d\xi d\eta$$
$$+ \int_{\hat{\Omega}(t-\epsilon)} [(UG)|_{\tau=t-\epsilon} - (UG)|_{\tau=t^*(\xi,\eta)}] d\xi d\eta$$
$$= \int_0^{t-\epsilon} \int_{\Gamma(\tau)} a^2 (G \frac{\partial U}{\partial n} - U \frac{\partial G}{\partial n}) d\sigma d\tau \qquad (2.17)$$

In equation (2.17), the last term on the left hand side and the second term on the right hand side vanish because U vanishes on $\Gamma(t)$. Thus,

$$\int_{\Omega(t-\epsilon)} UG|_{\tau=t-\epsilon} d\xi d\eta = \int_{\Omega(0)} G(x, y, t; \xi, \eta, 0) \phi(\xi, \eta) d\xi d\eta$$
$$+ \int_0^{t-\epsilon} \int_{\Gamma(\tau)} a^2 G \frac{\partial U}{\partial n} d\sigma d\tau \qquad (2.18)$$

We now choose G to be

$$G(x, y, t; \xi, \eta, \tau) = \frac{1}{4\pi a^2 (t-\tau)} e^{-[(x-\xi)^2 + (y-\eta)^2]/[4a^2(t-\tau)]} \qquad (2.19)$$

which is the two dimensional Green's function for the heat equation on an infinite domain. It is the solution of the heat equation with a Dirac delta source:

$$\frac{\partial G}{\partial t} = a^2\nabla^2 G + \delta(x-\xi)\delta(y-\eta)\delta(t-\tau) \tag{2.20}$$

The Green's function G is a solution of the adjoint equation (2.14) and if we take the limit as $\epsilon \to 0$ we obtain from equation (2.18)

$$\begin{aligned} U(x,y,t) = &\int_{\Omega(0)} G(x,y,t;\xi,\eta,0)\phi(\xi,\eta)d\xi d\eta \\ &+ \int_0^t \int_{\Gamma(\tau)} a^2 G \frac{\partial U}{\partial n_{\xi\eta}} d\sigma d\tau \end{aligned} \tag{2.21}$$

In equation (2.21) we have included a ξ,η subscript on the normal derivative $\partial/\partial n$ because we are now going to take the partial derivative of both sides of equation (2.21) with respect to the normal at (x,y). We take $\frac{\partial U}{\partial n_{x,y}}$, take the limit as $(x,y)\to\Gamma(t)$, and define $V(x,y,t)$ on $\Gamma(t)$ by $V(x,y,t)|_{\Gamma(t)} = \left.\frac{\partial U}{\partial n}\right|_{\Gamma(t)}$ then

$$\begin{aligned} V(x,y,t)|_{\Gamma(t)} = &\int_{\Omega(0)} \frac{\partial}{\partial n_{xy}} G(x,y,t;\xi,\eta,0)\phi(\xi,\eta)d\xi d\eta \\ &+\frac{1}{2}V(x,y,t)|_{\Gamma(t)} + \int_0^t \int_{\Gamma(\tau)} a^2 \frac{\partial G}{\partial n_{xy}} V d\sigma d\tau \end{aligned} \tag{2.22}$$

Note that, for the integral on $\Gamma(\tau)$, G and V are evaluated at $(x,y,t;\xi(\sigma,\tau),\eta(\sigma,\tau),\tau)$. Thus

$$\begin{aligned} V(x,y,t)|_{\Gamma(t)} = 2&\int_{\Omega(0)} \frac{\partial}{\partial n_{xy}} G\phi(\xi,\eta)d\xi d\eta \\ &+2a^2 \int_0^t \int_{\Gamma(\tau)} \frac{\partial G}{\partial n_{xy}} V d\sigma d\tau \end{aligned} \tag{2.23}$$

By integrating the last two equations from equations (2.9) we obtain the following two equations which describe how the boundary moves with time:

$$x_\sigma(t)|_{\Gamma(t)} = x_\sigma(0)|_{\Gamma(0)} - k_1 \int_0^t U_x(x,y,\tau)|_{(x_\sigma,y_\sigma)\in\Gamma(\tau)} d\tau \tag{2.24}$$

$$y_\sigma(t)|_{\Gamma(t)} = y_\sigma(0)|_{\Gamma(0)} - k_2 \int_0^t U_y(x,y,\tau)|_{(x_\sigma,y_\sigma)\in\Gamma(\tau)} d\tau \tag{2.25}$$

Here σ is an index that denotes the particular point on the boundary that is of interest. We use equation (2.24) to determine the x-coordinates of the trajectory of this boundary point designated by σ and we use equation (2.25) to determine the y-coordinates.

In order to solve for the temperature distribution on the domain and the position of the moving boundary, we will employ the following algorithm:

Algorithm 2:

1. Guess $V_0(x,y,t)|_\Gamma$, $x_0(x,y,t)|_\Gamma$, $y_0(x,y,t)|_\Gamma$.
2. Use $V_0(x,y,t)|_\Gamma$ in the right hand side of equation (2.23) to obtain $V_1(x,y,t)|_\Gamma$ from the left hand side of equation (2.23). Use $V_1|_\Gamma$ in (2.21) to calculate $U_x|_\Gamma, U_y|_\Gamma$. Use these values in (2.24) and (2.25) to obtain $x_1|_\Gamma$, $y_1|_\Gamma$.
3. Iterate until convergence.
4. Use converged values in (2.21) to obtain U.

In step (1), we generate the initial input for the method. In step (2), we apply the input to the system in order to give us a "better" estimate of the solution to the system. We then apply this better estimate to the system input in a feedback iteration loop in step (3). We repeat until the output from the system is within the accuracy envelope that we require. We then use the solutions we obtained for the moving boundary position and the heat flux in the equation for the temperature $U(x,y,t)$ in step (4).

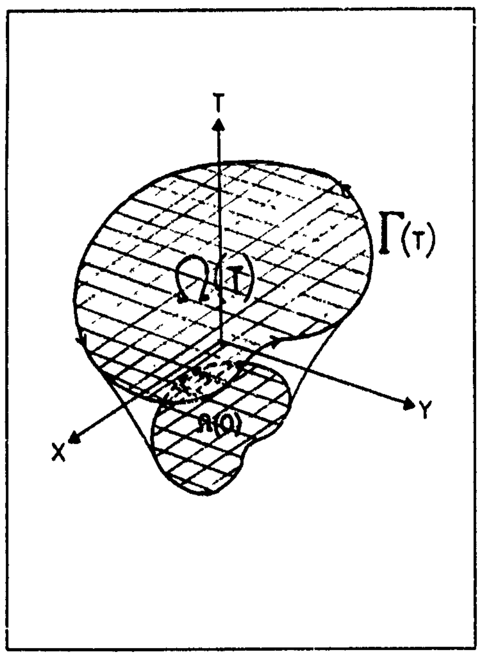


Figure 2.3. Domain for the Two Dimensional Problem

III. Results

3.1 Temperature and Moving Boundary Calculations

We choose the domain at time $t = 0$, $\Omega(0)$, to be the open disk $x^2 + y^2 < 0.36$ in the x-y plane. We also choose our initial condition $U(x, y, 0) = \phi(x, y) = J_0(c\sqrt{x^2 + y^2})$ where J_0 is the Bessel function of order zero. Here c is a constant that we need to determine. If we choose $k_1 = k_2 = 0$ in equation (2.9) and thereby let the boundary be fixed, we will have a well-posed two dimensional initial-boundary value problem for the heat equation. This problem can be solved by the method of separation of variables to yield the solution

$$U(x, y, t) = \exp(-2c^2 t) J_0(c\sqrt{x^2 + y^2})$$

for the cylindrically symmetric fixed domain $\Omega(t) = \Omega(0)$, $t > 0$. The boundary condition requires the temperature to be equal to zero on the boundary of the domain for all values of time. Therefore, the above equation for $U(x, y, t)$ is a solution if $0.6c$ is the smallest zero of the Bessel function J_0. The smallest zero of J_0 is equal to 2.4048256 and we thus determine that c is equal to 4.0080426. If we substitute this value for c into our expression for the temperature, we will obtain the initial temperature surface shown in Figure (3.1). If we now allow time to progress from $t = 0$ to $t = 0.225$, we will obtain the series of heat surfaces shown in Figures (A.1) and (A.2). The exponential decay with respect to time is readily apparent in the figures. Also, note that the boundary does not move as time progresses. We now look at the above solution for the fixed boundary problem at the points shown in Table (3.1) and also at the origin (0, 0). We allow t to take on the values in the interval $0 \leq t \leq 0.3$. The solution at the given points is shown by the solid curves in Figure (3.2). Curve A is the solution $U(x, y, t)$ as a function of time at the origin (0, 0). Curve B is $U(x, y, t)$ for (x, y) being any of the eight points of group B in

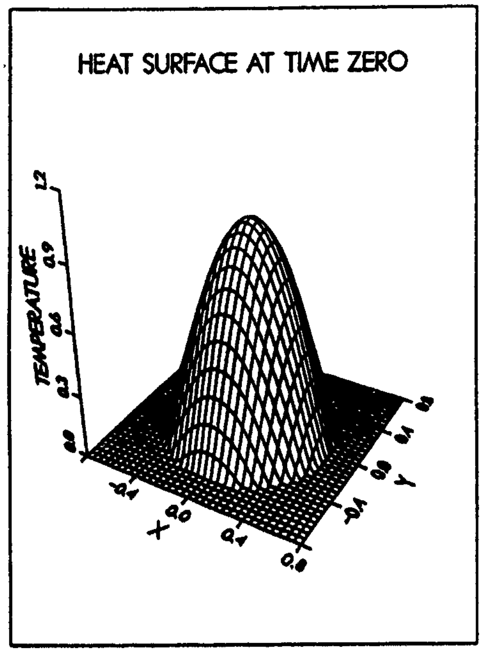


Figure 3.1. Initial Condition Temperature Surface

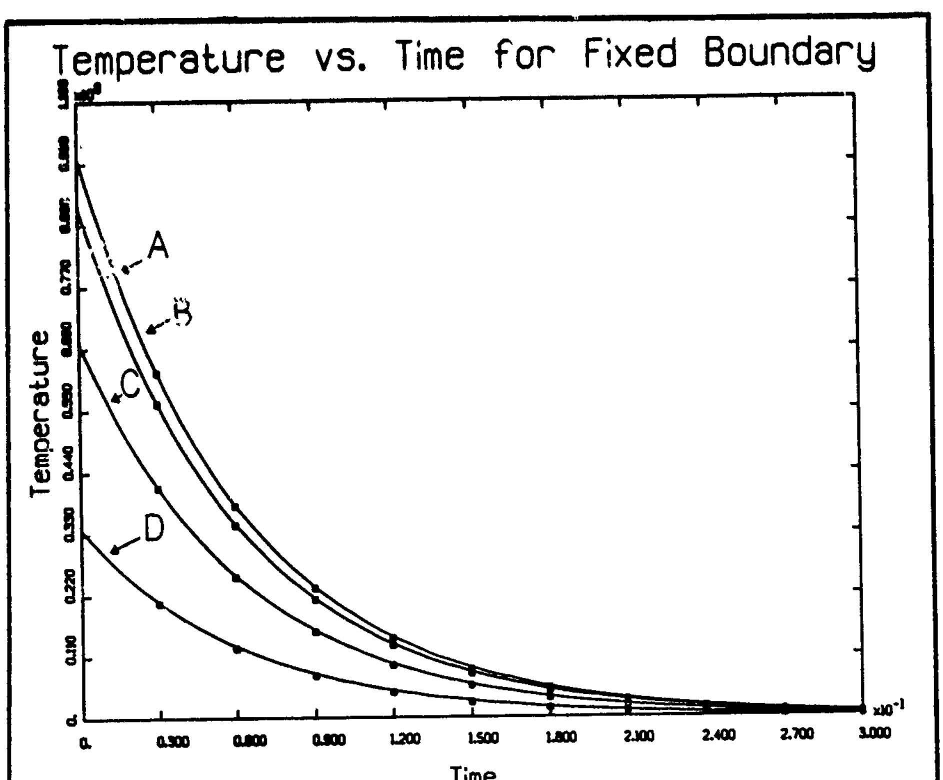


Figure 3.2. Solution for a Fixed Boundary

Point Number	Angle(radians)	X-Coordinate	Y-Coordinate	
1	0.	0.1500000	0.	
2	0.7853981	0.1060660	0.1060660	
3	1.5707963	0.0000000	0.1500000	
4	2.3561945	-0.1060660	0.1060660	
5	3.1415927	-0.1500000	-0.0000000	B
6	3.9269910	-0.1060660	-0.1060660	
7	4.7123890	0.0000000	-0.1500000	
8	5.4977870	0.1060660	-0.1060660	
1	0.	0.3000000	0.	
2	0.7853981	0.2121321	0.2121320	
3	1.5707963	0.0000000	0.3000000	
4	2.3561945	-0.2121320	0.2121320	
5	3.1415927	-0.3000000	-0.0000000	C
6	3.9269910	-0.2121320	-0.2121321	
7	4.7123890	0.0000000	-0.3000000	
8	5.4977870	0.2121320	-0.2121321	
1	0.	0.4500000	0.	
2	0.7853981	0.3181981	0.3181981	
3	1.5707963	0.0000000	0.4500000	
4	2.3561945	-0.3181981	0.3181981	
5	3.1415927	-0.4500000	-0.0000000	D
6	3.9269910	-0.3181980	-0.3181981	
7	4.7123890	0.0000000	-0.4500000	
8	5.4977870	0.3181980	-0.3181981	

Table 3.1. Solution Evaluation Points

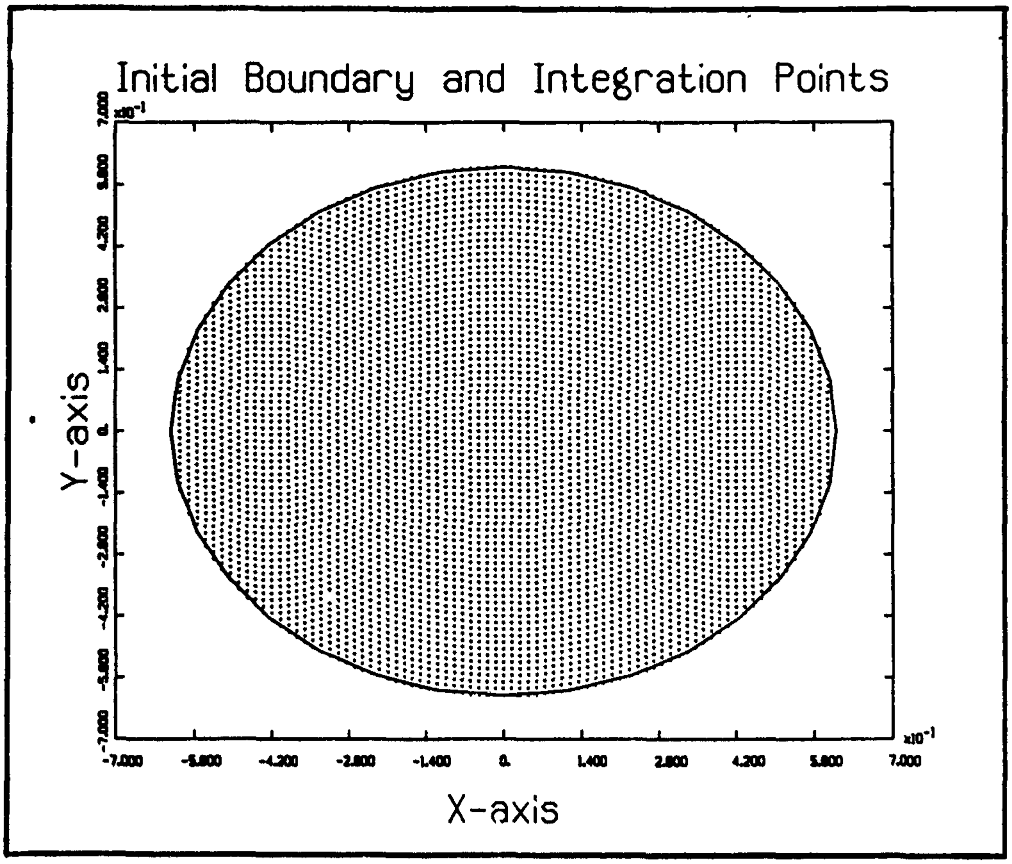


Figure 3.3. Domain Increments Used for Integration

Table (3.1). The plot of the solution for each point repeats on the same curve due to the symmetry of the problem. Curve C is $U(x,y,t)$ at the eight points shown in group C in the table. And finally, curve D is $U(x,y,t)$ at the eight points shown in group D. We now use our algorithm to solve the fixed boundary problem. We evaluate the integral over $\Omega(0)$ in equation (2.23) by dividing the x-axis into 80 increments. This will result in a division of the y-axis which is allotted proportionally as we move across the domain along the x-axis. We used this proportional spacing to save computation time. It is unnecessary to use a very fine grid as we are integrating over y when the length of the y-segment is short, as occurs towards the outer edges of the domain as viewed along the x-axis. This is completely due to the specific geometry we have chosen for our domain. If we had chosen a square, then the y-axis would be broken up into the same number of increments as the x-axis. We break the boundary into 32 boundary elements, and the time axis into 100 increments. The spatial division of the domain is shown in Figure (3.3). We now iterate 12 times to reach

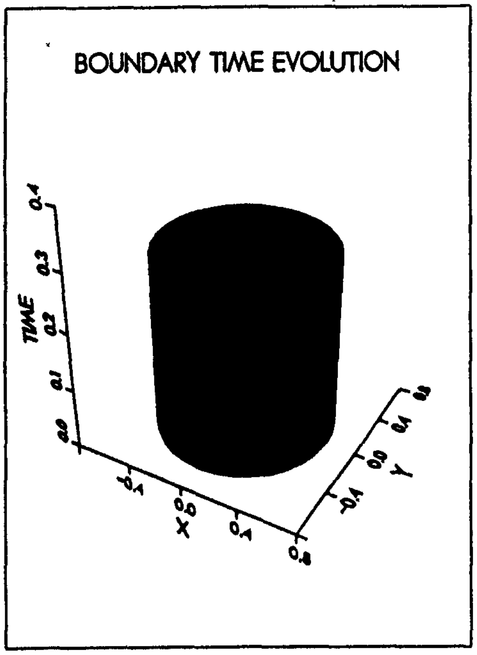


Figure 3.4. Fixed Boundary Time Evolution

convergence in the successive approximation. The squares in Figure (3.2) represent the solution at selected time values, again at the above selected spatial points, using our algorithm. The squares fall on or very close to the curves which represent the theoretical solution. We will analyze the errors later. If we draw a three-dimensional graph showing the boundary time evolution for the fixed boundary, we will have the result shown in Figure (3.4). The vertical lines show the time trajectories of the boundary points used in calculating the boundary integral around the fixed boundary. The circles represent the boundary at each moment of time.

We next use our algorithm to solve the moving boundary problem corresponding to $k_1 = k_2 = 1.0$ in equation (2.9). For this moving boundary problem, we iterated 11 times to obtain the solution indicated in Figure (3.5). The curves in Figure (3.5) are the same curves that appear in Figure (3.2) and thus they represent the theoretical solution. They are included for reference to compare the solution of the moving boundary problem with the solution of the theoretical fixed boundary problem. The squares in Figure (3.5) represent the solution obtained using our algorithm at the same points as the data points in Table (3.1). The squares which

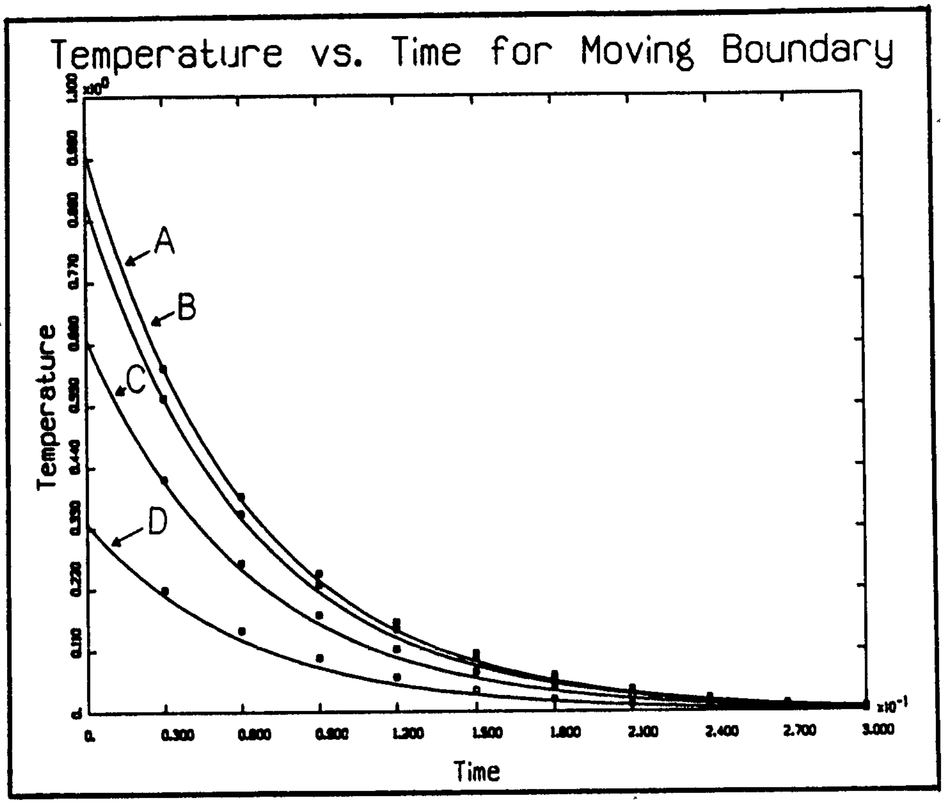


Figure 3.5. Solution for Moving Boundary with $k_1 = k_2 = 1.0$

indicate our solution of the moving boundary problem show a shift as the boundary moves which is as we would expect. The temperature is higher at a specific point at a given time since the boundary of the domain is moving outward from the center of the domain. The boundary time evolution for the moving boundary is shown in Figure (3.6). Again, the vertical lines show the time trajectories of the boundary points used in calculating the the boundary integral around the moving boundary. If we look at the motion of the boundary in two dimensions, we will obtain the graph shown in Figure (3.7). The decay of the temperature surface with respect to time is shown in the series of graphs in Figures (A.3) and (A.4). We can see that the temperature falls off at a faster than linear rate and that the surface spreads out as the boundary expands. The expansion rate is equal in the x- and y-directions.

We now will allow different expansion rates in the x- and y-directions. We set $k_1 = 3.0$ and $k_2 = 0.5$. We obtain convergence after 12 iterations. The expanding boundary will be graphed as shown in Figure (3.8). It is readily apparent that the

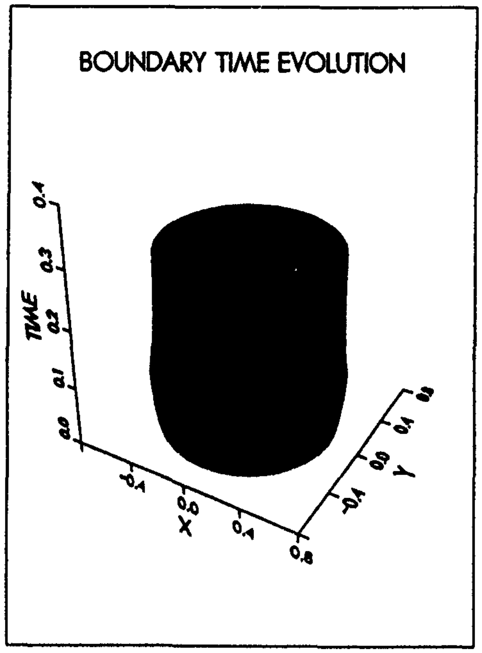


Figure 3.6. Moving Boundary Time Evolution

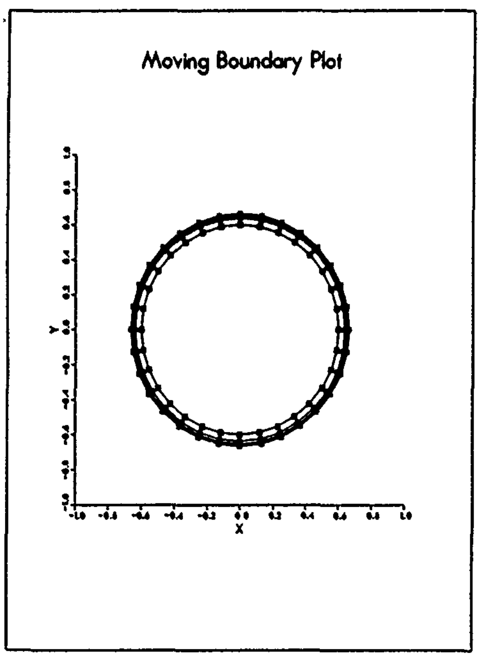


Figure 3.7. Moving Boundary for $k_1 = 1.0$ and $k_2 = 1.0$

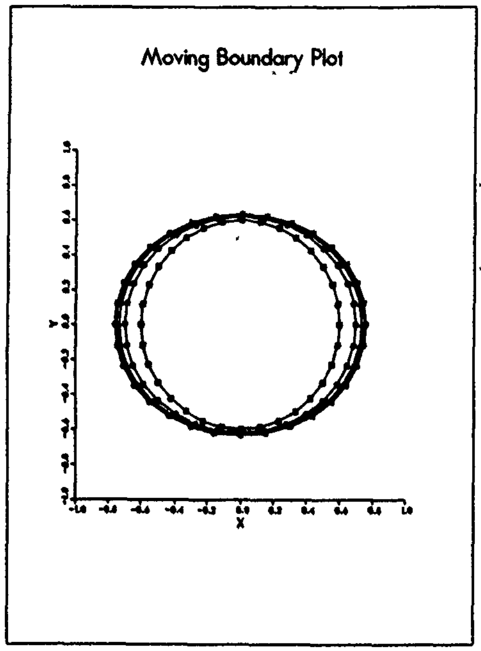


Figure 3.8. Moving Boundary for $k_1 = 3.0$ and $k_2 = 0.5$

boundary is moving much more in the x-direction than in the y-direction. This case is no longer cylindrically symmetric and hence represents a true two-dimensional solution of the heat equation. The decay of the temperature surface is shown in Figures (A.5) and (A.6). We can see the greater broadening of the surface in the x-direction than in the y-direction.

For added emphasis of the different expansion rates, we set $k_1 = 5.0$ and $k_2 = 0.5$. The two-dimensional moving boundary is shown in Figure (3.9). The expansion in the x-direction is very pronounced. The three-dimensional boundary time evolution for the moving boundary is shown in Figure (3.10). The temperature surfaces are shown in Figures (A.7) and (A.8). Here the surface becomes much thinner in the y-direction as time progresses.

3.2 *Execution Times*

The execution times were determined as a function of both the division of the time axis and the division of the space axes. The division of the boundary was allowed

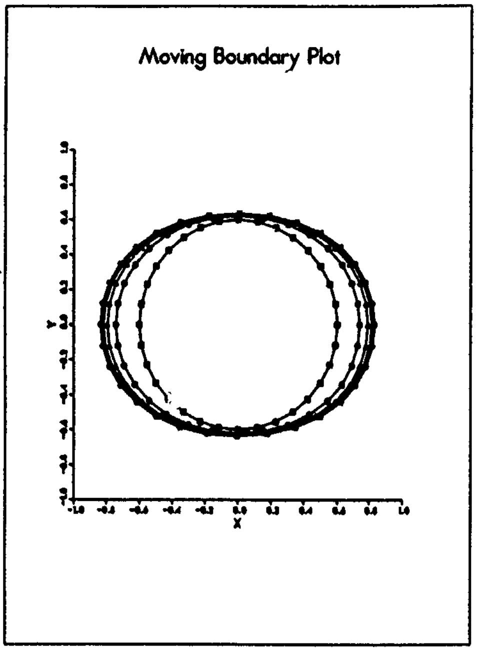


Figure 3.9. Moving Boundary for $k_1 = 5.0$ and $k_2 = 0.5$

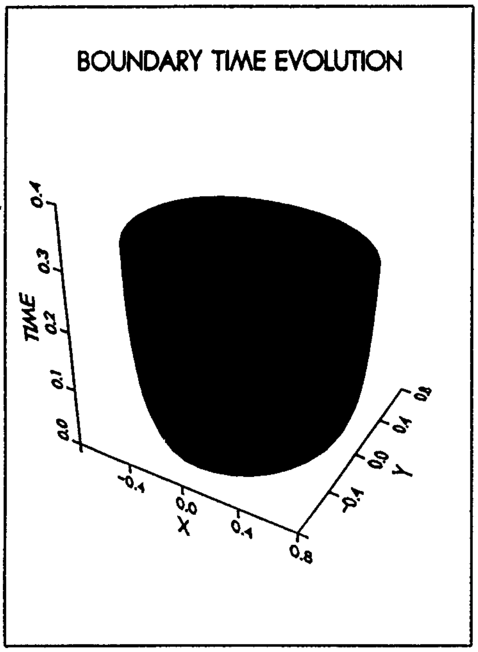


Figure 3.10. Moving Boundary Time Evolution for $k_1 = 5.0$ and $k_2 = 0.5$

to vary from $nps = 22$ to $nps = 32$ points in increments of two elements. The three-dimensional plots of the execution times are shown in Figures (A.9) and (A.10).The execution times as a function of the division of the time axis, nt, are shown in Figures (A.11) and (A.12). Here we notice that the execution time increases almost linearly with respect to nt. We expect this since the time division will determine the amount of time spent in the integration loop for the line integral and this is a single loop as opposed to the nested loop for the spatial integrations. The execution times as a function of the division of the space axes is shown in Figures (A.13) and (A.14). Here one must remember that the division of the y-axis is dependent upon the division of the x-axis. Therefore, the label "nx" actually represents the compound effect of the division of both space axes. This is why the growth of the execution time curve is geometric with respect to nx. The spatial integrations are performed by a nested loop which effectively represents the product of the spatial dimensions, thereby reflecting a quadratic growth rate. Thus we see that the execution times are almost independent of the number of boundary elements and that they depend most strongly on the spatial division of the domain. Therefore, in order to keep computational time to a minimum, it is advisable to keep nx as small as possible and still retain the accuracy that we require. We can allow nps to be larger since it has a smaller effect on the execution time. The value of the time division, nt, will determine the execution time at an intermediate rate. We can consult the graphs and pick values that give reasonable execution times for the accuracy that we require. The execution times given are all for the ELXSI computer of the Air Force Institute of Technology.

IV. Conclusions and Recommendations

4.1 Satisfaction of Goals

We have presented the mathematical derivation of models for phase change problems in one and two dimensions using the boundary element technique. We then applied this boundary element technique to a specific series of two dimensional melting ice problems. We note that our models are also applicable to the solution of the diffusion equation. This thesis has amply demonstrated the facility of using computer graphics as a tool to display numerical results. The sheer volume of the results from the calculations would overwhelm our ability to see the patterns of meaning without the use of computer graphics.

4.2 Future Work

This research is ripe for further development. Viable areas for further work include:

- Consider other two dimensional domains on which to solve the heat equation. These could include:

    1. Convex and non-convex shapes.

    2. Symmetric and non-symmetric shapes.

- Extend the problem to three dimensions. For a development of the three dimensional equations that is similar to our development in this thesis, see (11:105–110).

- Allow the medium to become non-homogeneous or anisotropic. This implies allowing K_0, c, and ρ to be spatially-dependent.

- Change the boundary conditions. Possible changes include:

1. Allow the temperature to be non-zero along parts of the boundary (non-homogeneous problem).

2. Insulate parts of the boundary (Neumann condition).

3. Allow mixed or Robin boundary conditions along parts of the boundary.

- Make the problem non-homogeneous by allowing sources and/or sinks of heat energy within the domain.
- Allow the medium properties K_0, c, and ρ to be time-dependent.
- Utilize alternate methods, such as Gaussian quadrature, for performing the numerical integrations.
- Use other numerical methods, such as finite differences or finite elements, to solve the Stefan problem.
- Perform an execution time comparison and analysis between the solutions using alternate numerical methods.
- Perform an error comparison and analysis between the solutions using alternate numerical methods.
- Establish the contractive nature of the mapping for the two and three dimensional problems.

4.3 Remarks

We would recommend that effort be given to finding a numerically efficient method for performing the integrations used in solving the moving boundary problems. This thesis required an enormous amount of computer time. Further thought must be given to improving the execution speed and the memory requirements of the code, especially if more intricate geometries are to be considered. If fast computing resources are not available, the moving boundary problem becomes a formidable computational task. Also, the data files generated are rather large and it is not

possible to keep many of them on disk storage. Tape storage is one possibility. Also, further thought could be given to reducing the amount of required information to a minimum. We kept only recent results, but, found later that it would be advantageous to be able to refer back to earlier data. The computer graphics files also require a large amount of storage space.

Overall, this problem is quite intriguing and also satisfying. It is possible to obtain good results that fit well with one's intuitive expectations. Our appetite has certainly been whetted, and we would like to consider future work in this interesting area.

Appendix A. *Figures*

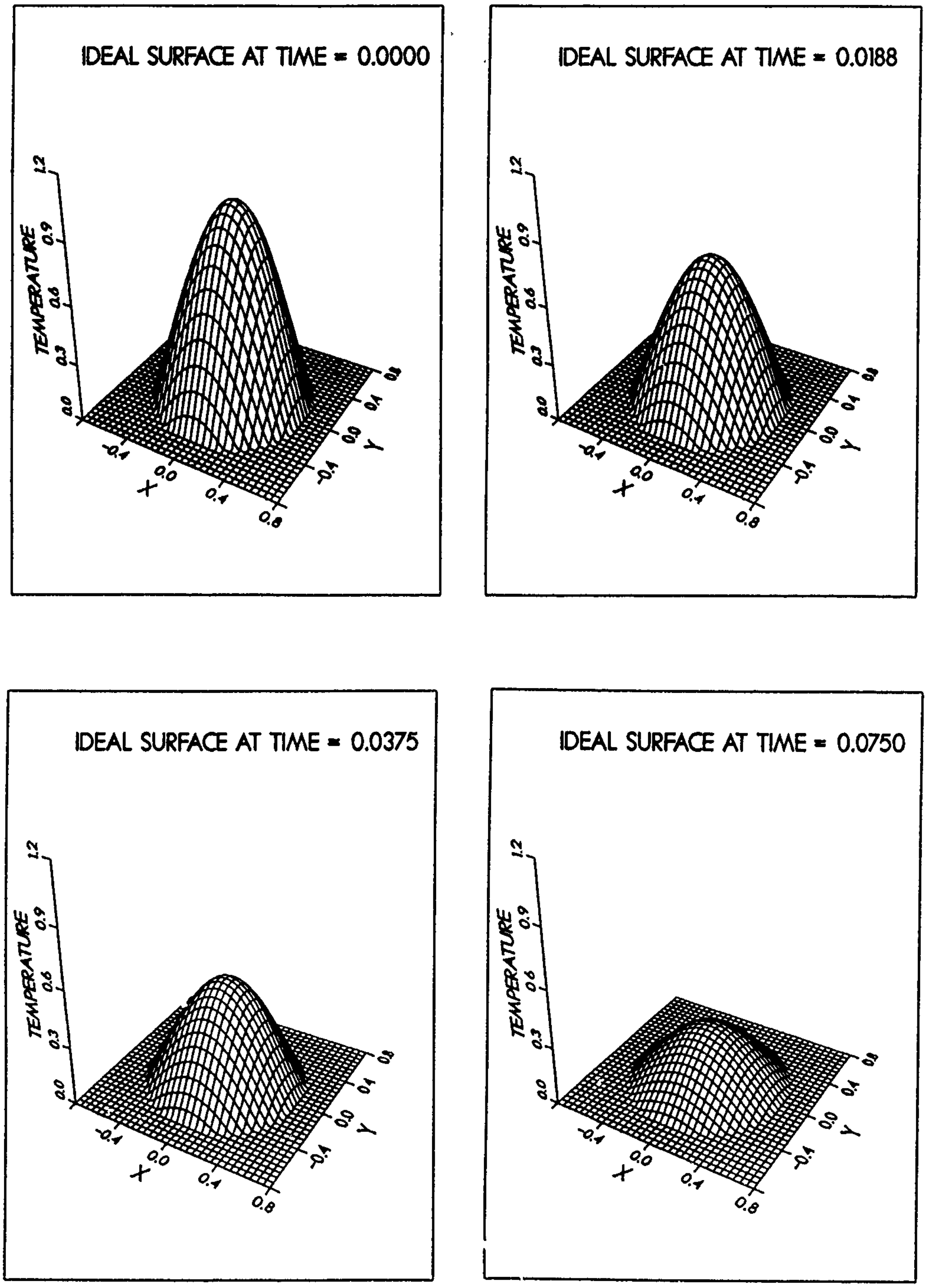


Figure A.1. Temperature Surfaces for Exact Solution (1 of 2)

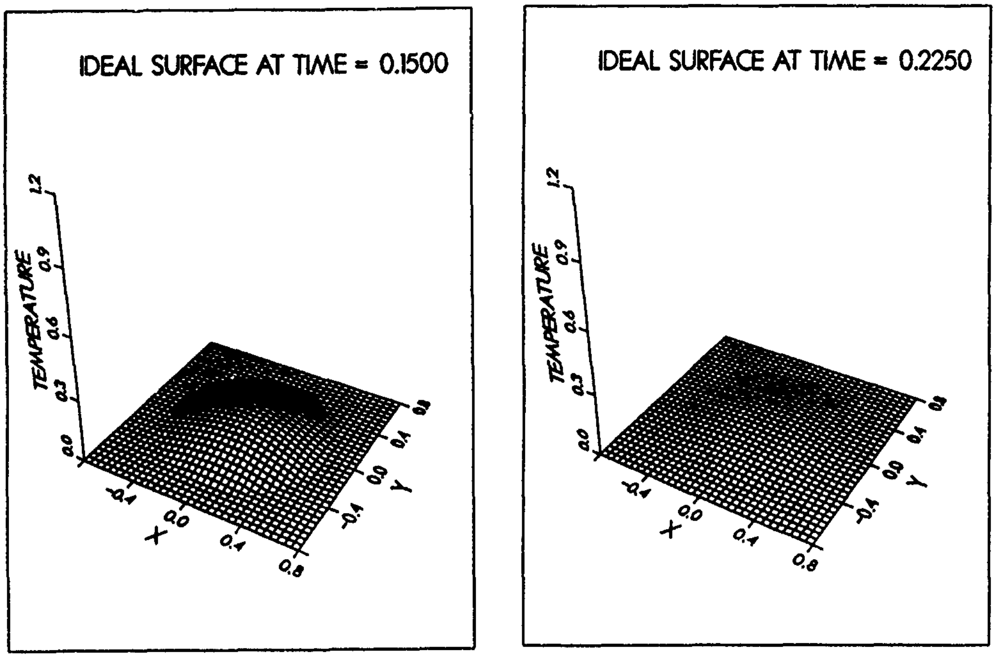


Figure A.2. Temperature Surfaces for Exact Solution (2 of 2)

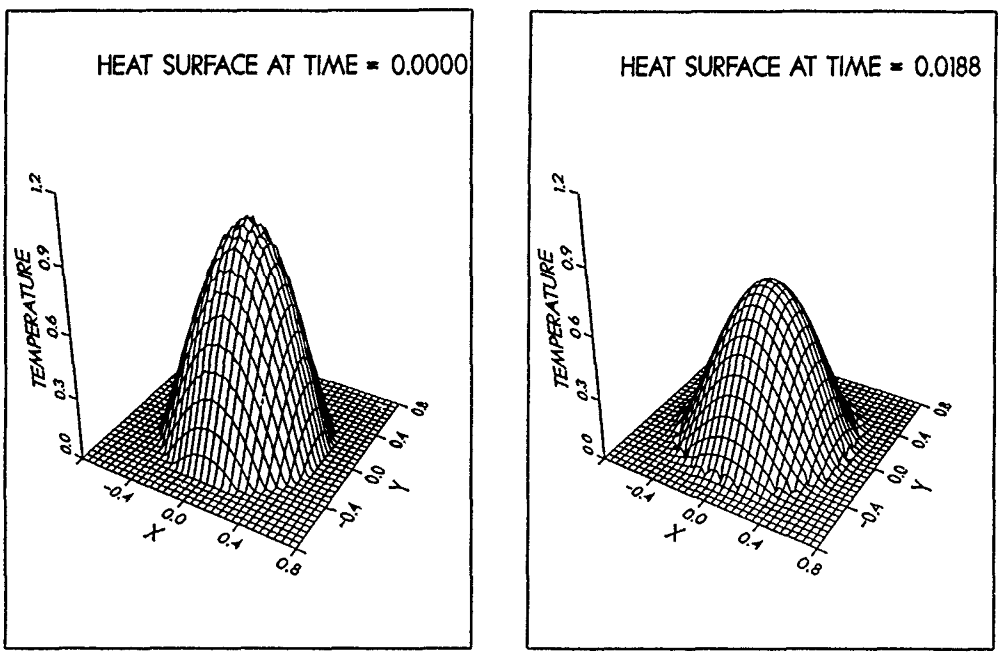


Figure A.3. Temperature Surfaces for $k_1 = 1.0$ and $k_2 = 1.0$ (1 of 2)

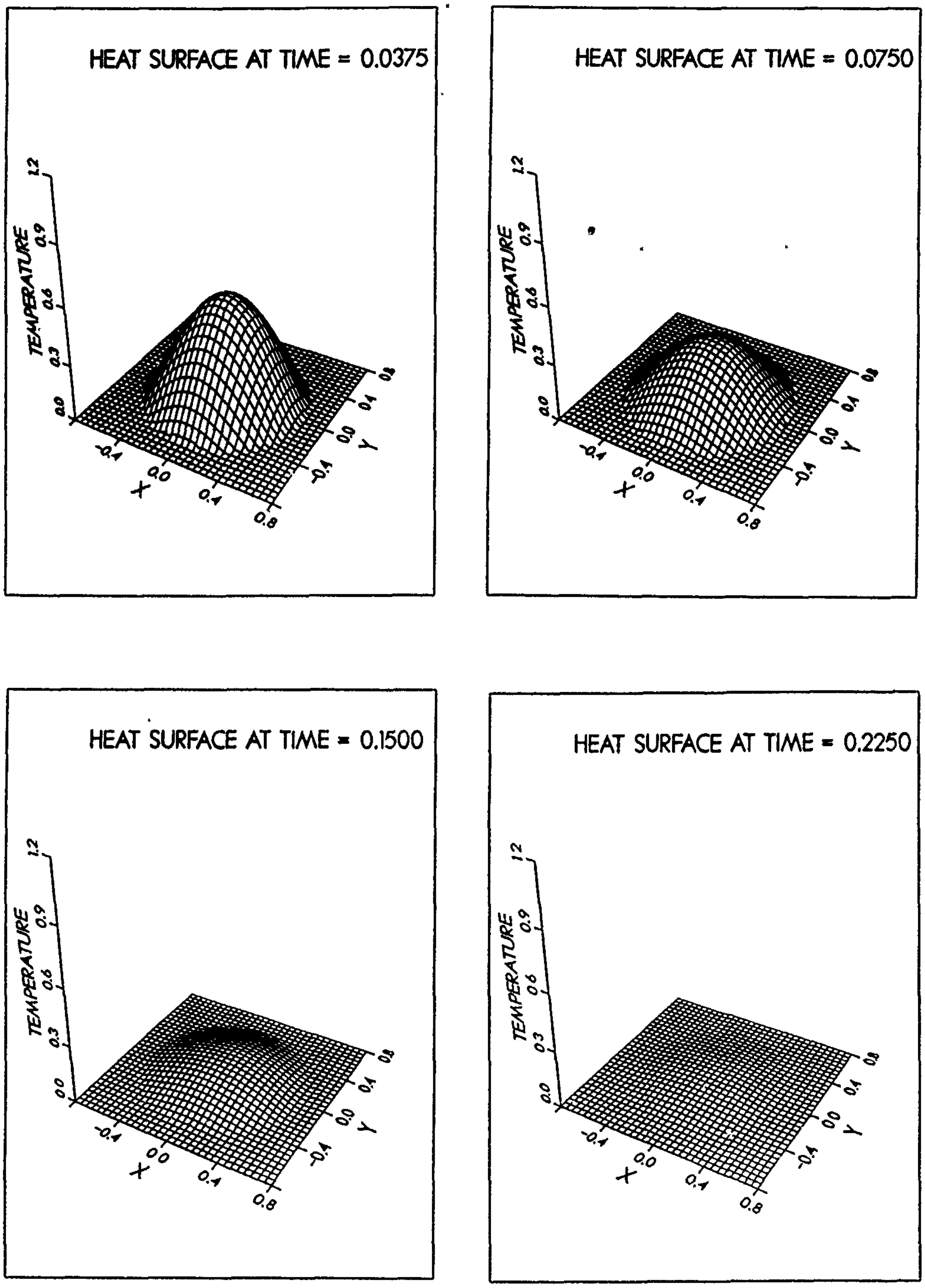


Figure A.4. Temperature Surfaces for $k_1 = 1.0$ and $k_2 = 1.0$ (2 of 2)

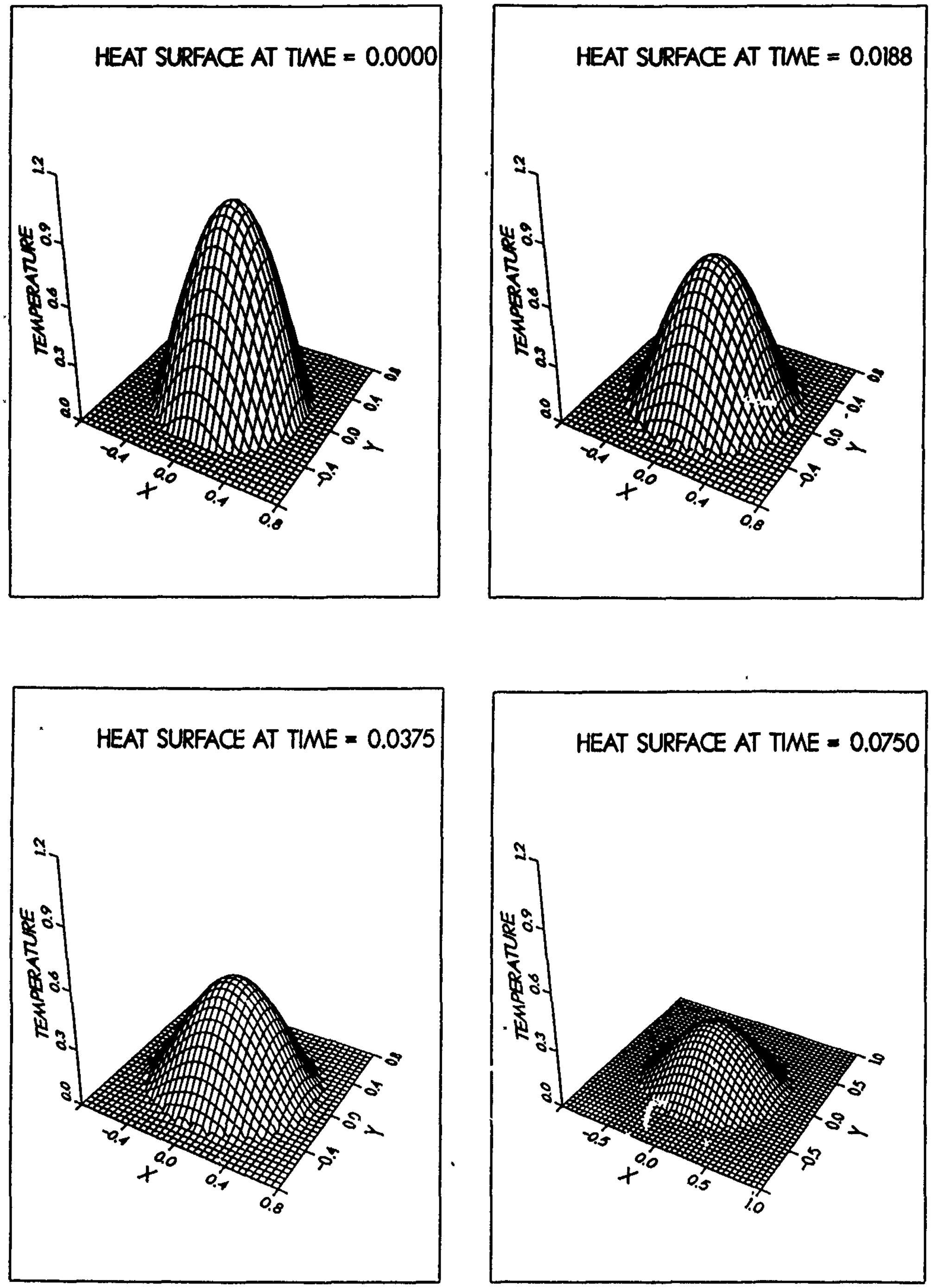


Figure A.5. Temperature Surfaces for $k_1 = 3.0$ and $k_2 = 0.5$ (1 of 2)

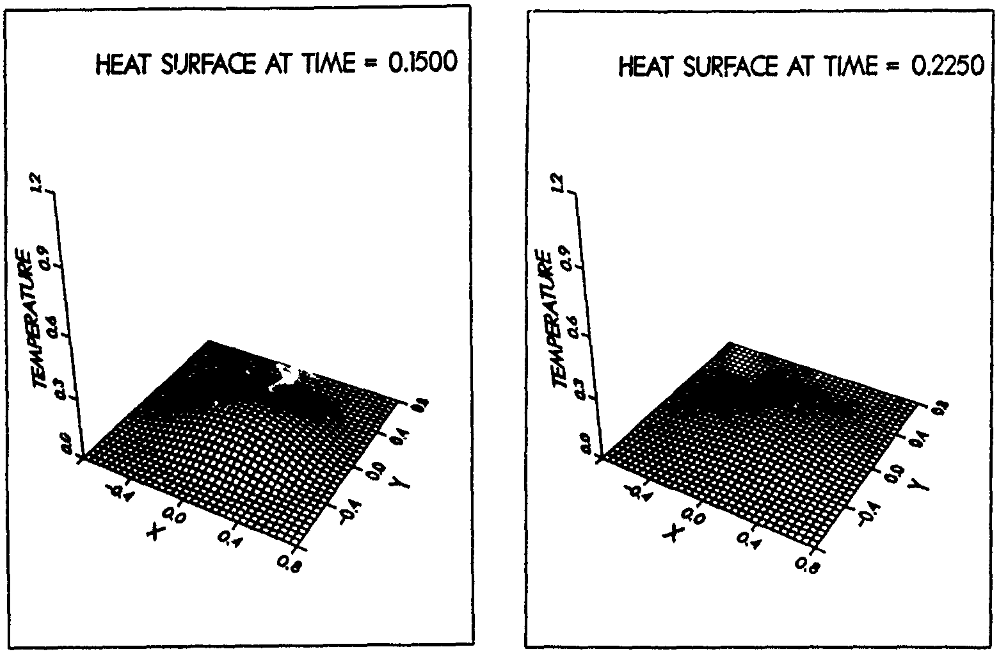


Figure A.6. Temperature Surfaces for $k_1 = 3.0$ and $k_2 = 0.5$ (2 of 2)

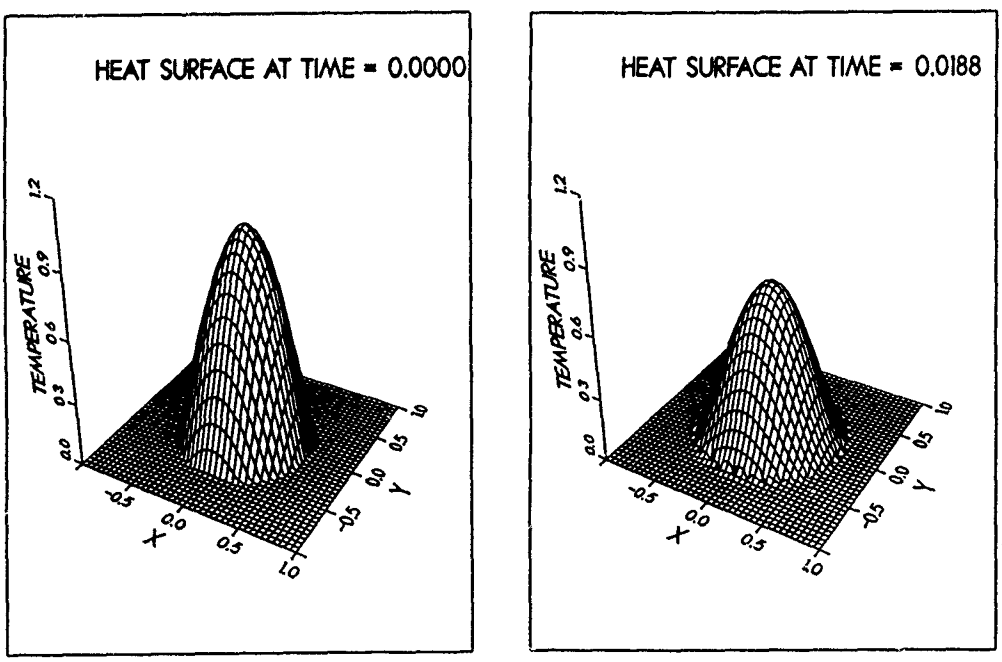


Figure A.7. Temperature Surfaces for $k_1 = 5.0$ and $k_2 = 0.5$ (1 of 2)

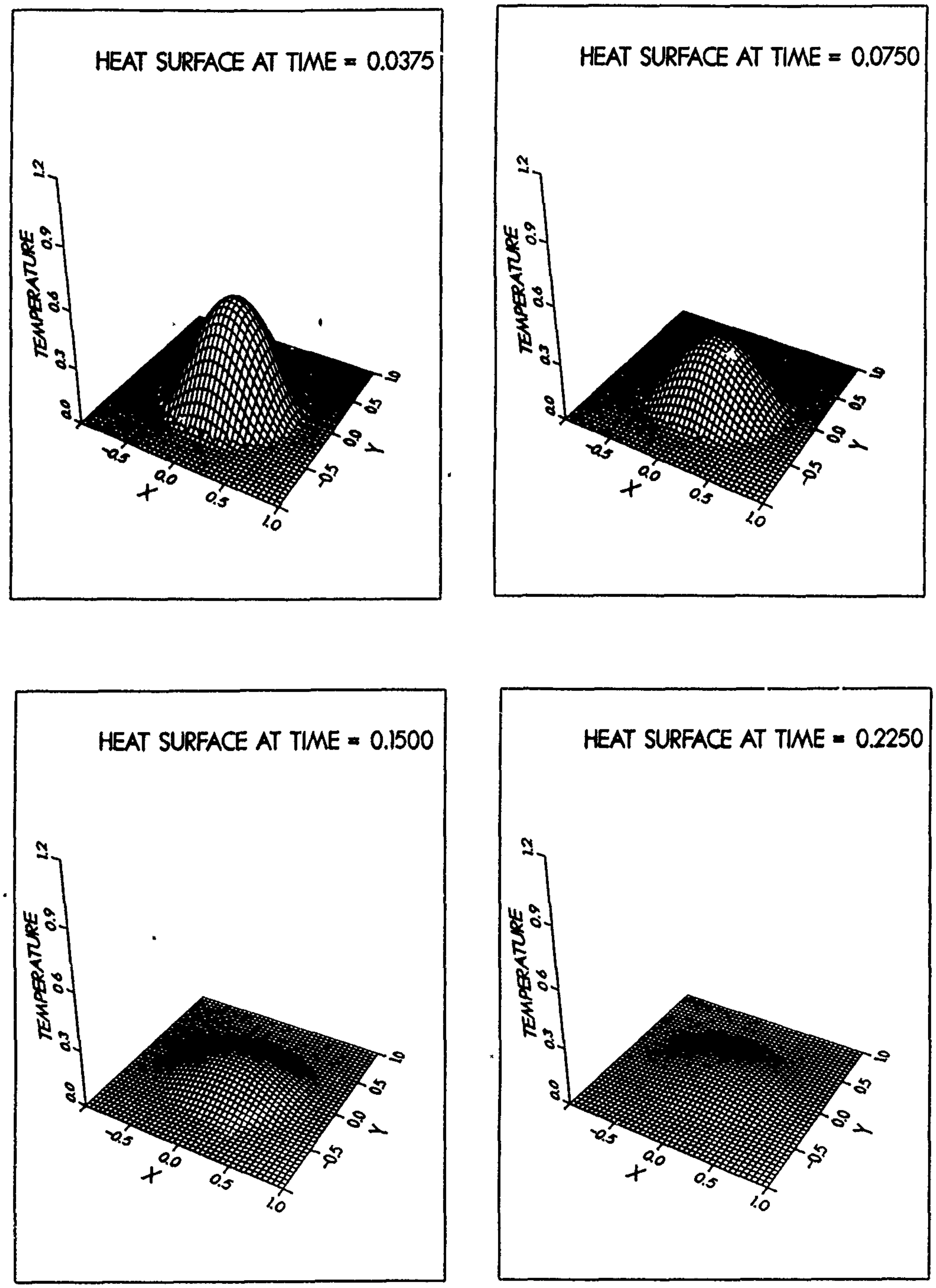


Figure A.8. Temperature Surfaces for $k_1 = 5.0$ and $k_2 = 0.5$ (2 of 2)

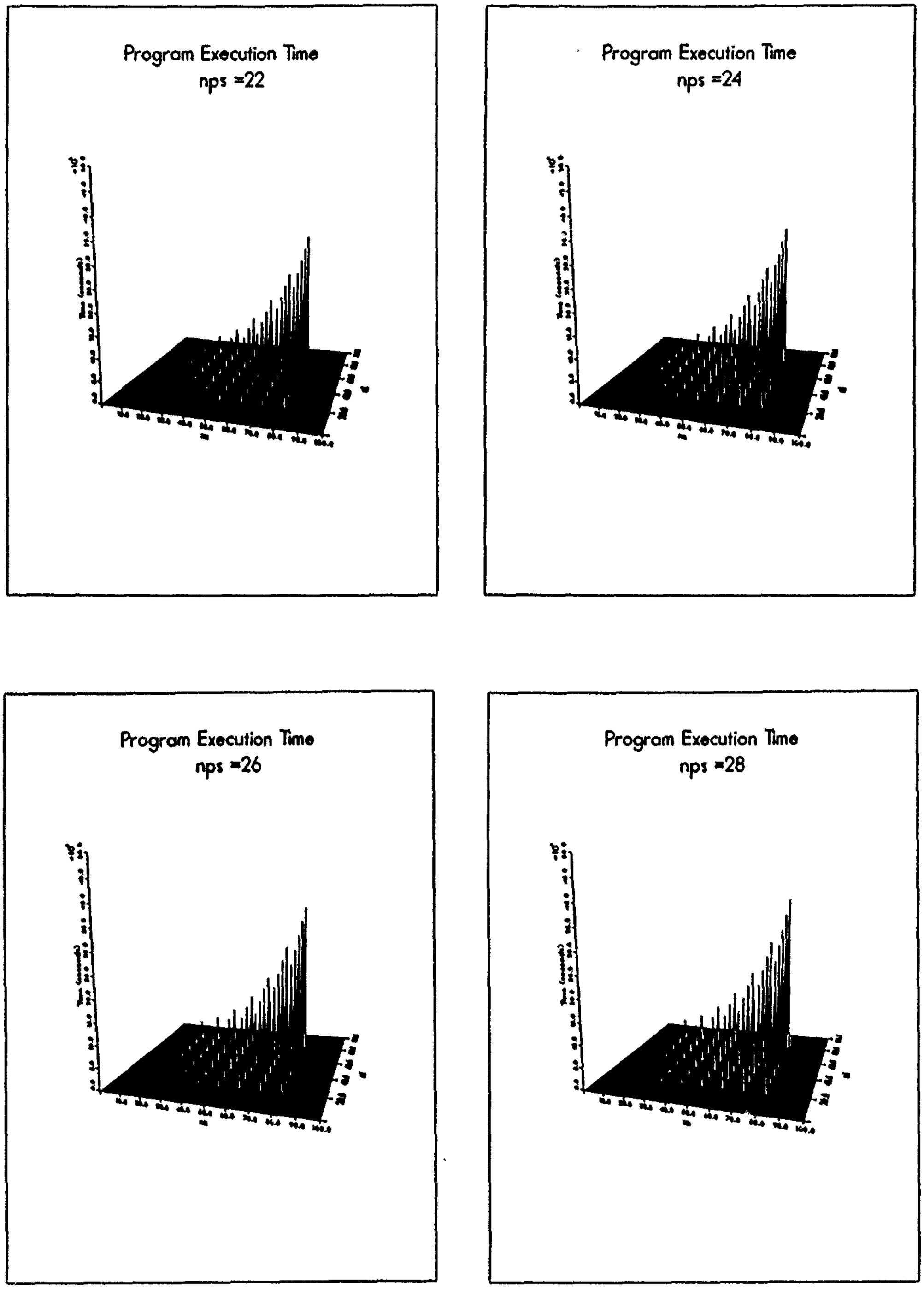
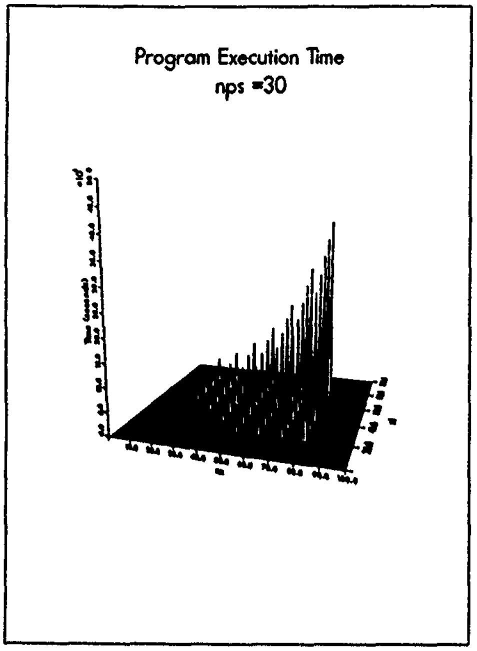


Figure A.9. Three Dimensional Plot of Execution Times (1 of 2)



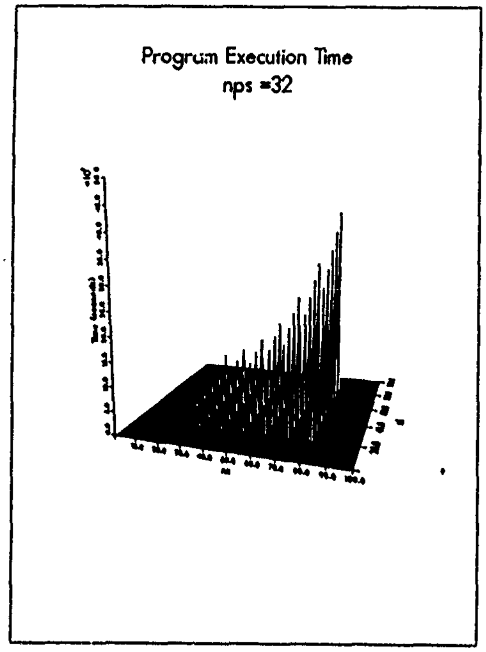
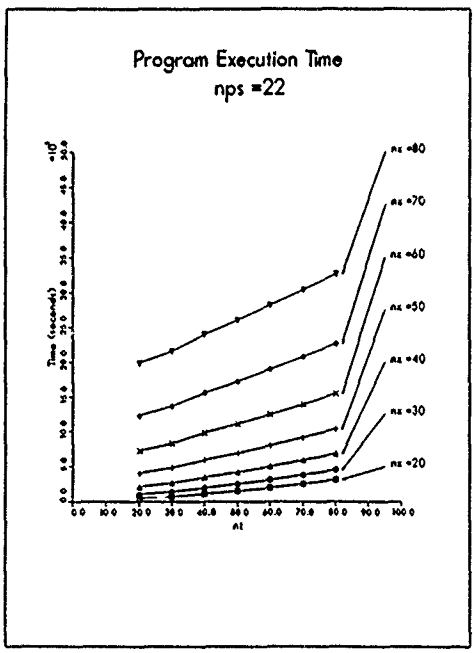


Figure A.10. Three Dimensional Plot of Execution Times (2 of 2)



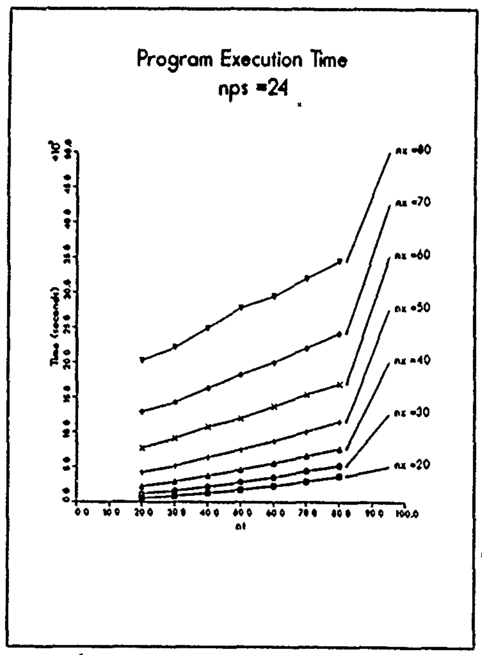


Figure A.11. Execution times as a function of nt (1 of 2)

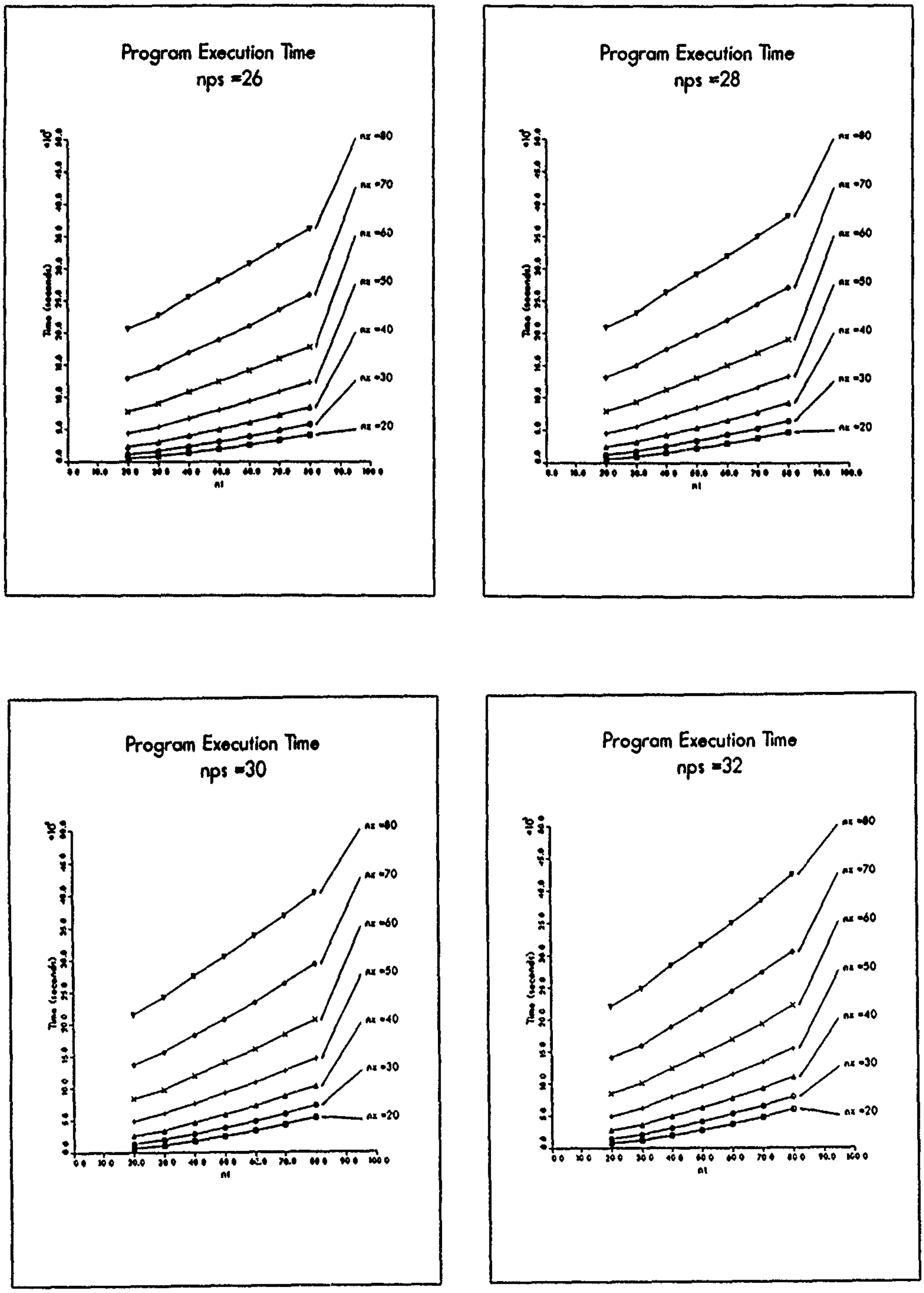


Figure A.12. Execution times as a function of nl (2 of 2)

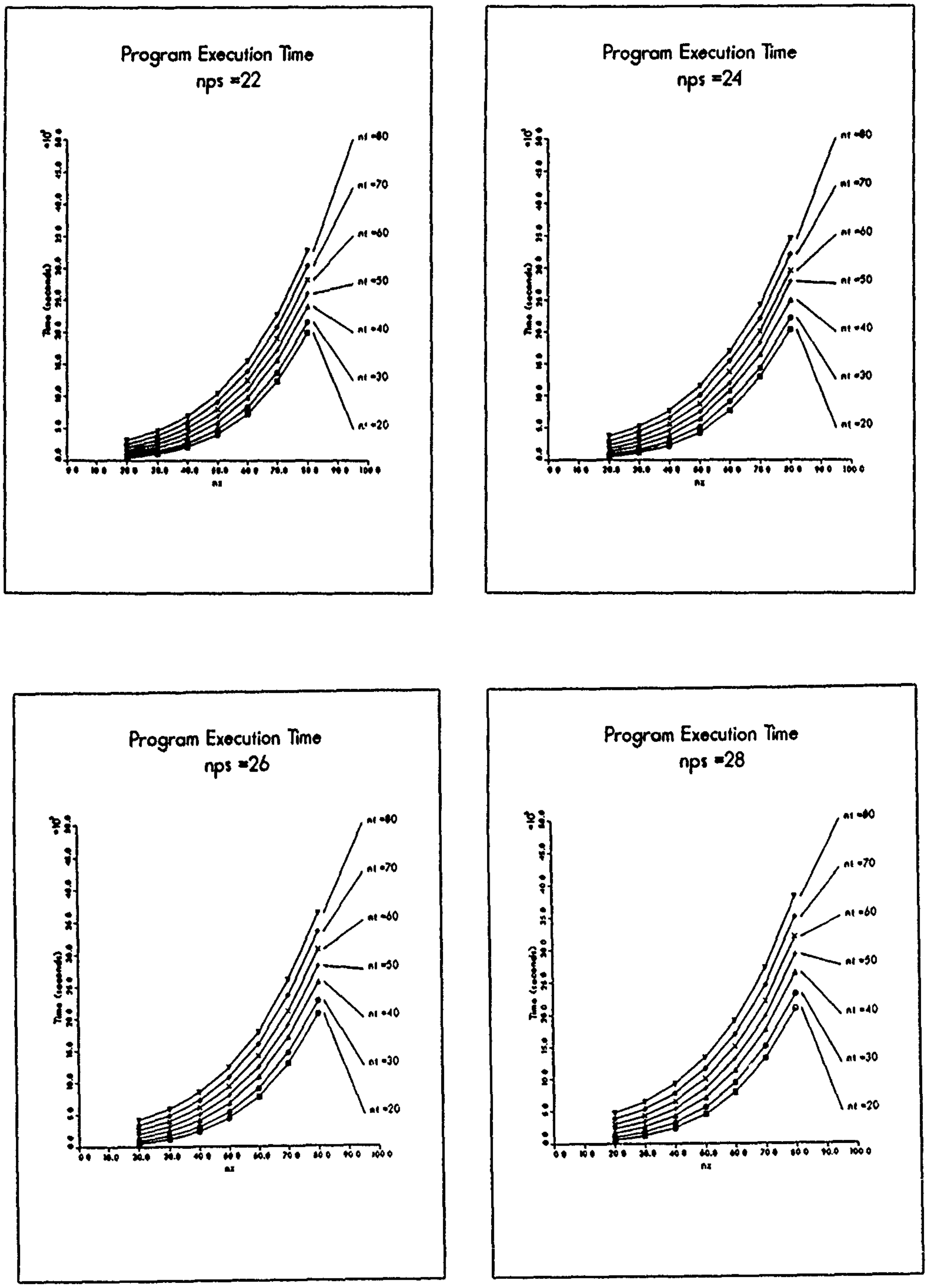


Figure A.13. Execution times as a function of nx (1 of 2)

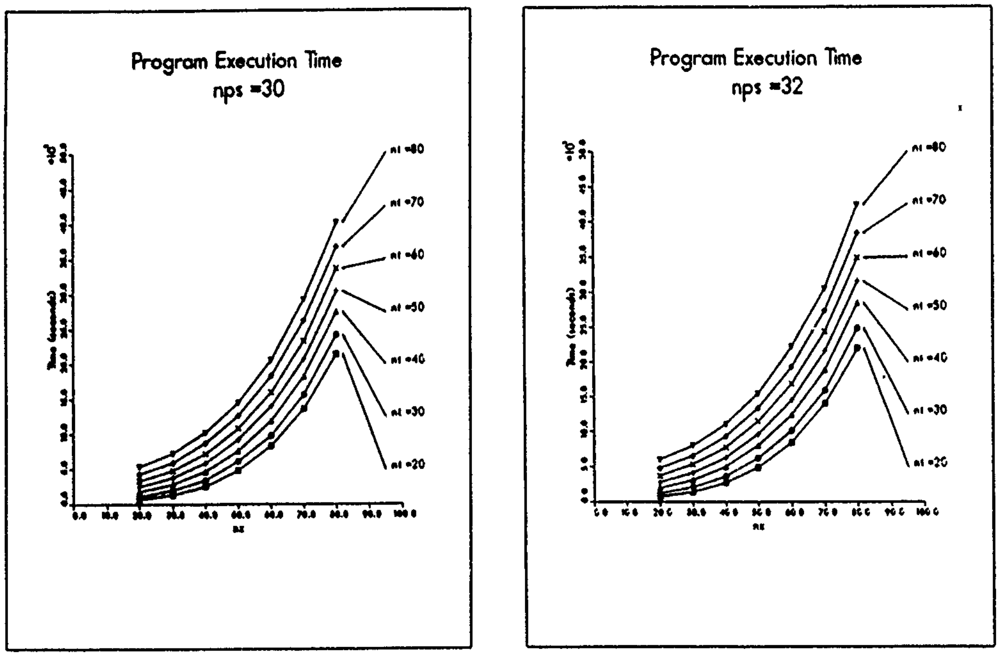


Figure A.14. Execution times as a function of nx (2 of 2)

Appendix B. *Derivation of the Limit*

We want to show, for $v(t)$ $(0 \leq t \leq \sigma)$ a continuous function, and the moving boundary $s(t)$ $(0 \leq t \leq \sigma)$ satisfying a Lipschitz condition, that for every $0 < t \leq \sigma$

$$\lim_{x-s(t)\to 0} \frac{\partial}{\partial x} \int_0^t v(\tau) K(x,t;s(\tau),\tau)d\tau = \frac{1}{2}v(t) + \int_0^t v(\tau) \left[\frac{\partial}{\partial x} K(x,t;s(\tau),\tau)\right]_{x=s(t)} d\tau$$

Here we have used the fundamental solution to the heat equation defined by:

$$K(x,t;\xi,\tau) = \frac{1}{2\pi^{1/2}(t-\tau)^{1/2}} e^{-\left\{\frac{(x-\xi)^2}{4(t-\tau)}\right\}}$$

In the following C_i, where i is an integer, denotes a constant. We start by defining the integral I:

$$I \equiv \int_{t-\delta}^{t} \frac{x-s(\tau)}{2(t-\tau)} K(x,t;s(\tau),\tau)d\tau - \int_{t-\delta}^{t} \frac{s(t)-s(\tau)}{2(t-\tau)} K(s(t),t;s(\tau),\tau)d\tau$$

We can write I as the sum of two other integrals, I_1 and I_2, where

$$I_1 = \int_{t-\delta}^{t} \frac{x-s(t)}{2(t-\tau)} K(x,t;s(\tau),\tau)d\tau$$

and

$$I_2 = \int_{t-\delta}^{t} \frac{s(t)-s(\tau)}{2(t-\tau)} \left[K(x,t;s(\tau),\tau) - K(s(t),t;s(\tau),\tau)\right] d\tau$$

The Lipschitz condition on the boundary $s(t)$ gives us

$$|s(t) - s(\tau)| < C_1|t-\tau|$$

This implies that

$$|I_2| \leq C_1 \int_{t-\delta}^{t} \frac{d\tau}{(t-\tau)^{1/2}} = 2C_1\delta^{1/2}$$

so $|I_2|$ will go to zero as δ goes to zero. We now want to look at $|I_1|$ and in order to do so we introduce the integral J_1 defined by

$$J_1 \equiv \int_{t-\delta}^{t} \frac{x - s(t)}{2(t-\tau)} K(x, t; s(t), \tau) d\tau$$

If we make the substitution $z = (t-\tau)/(x - s(t))^2$ in J_1 and note that $x - s(t) < 0$, we will have

$$J_1 = -\frac{1}{4\pi^{1/2}} \int_0^{\zeta} z^{-3/2} e^{-[1/4z]} dz$$

Here $\zeta = \delta/(x - s(t))^2$. When $x \to s(t)$ then $\zeta \to \infty$. Evaluating the integral for J_1 we see that $J_1 \to -\frac{1}{2}$. We look at $J_1 - I_1$

$$J_1 - I_1 = \int_{t-\delta}^{t} \frac{x - s(t)}{2(t-\tau)} K(x, t; s(t), \tau) \left[1 - e^{-\left\{ \frac{(x - s(\tau))^2 - (x - s(t))^2}{4(t-\tau)} \right\}} \right] d\tau$$

If we expand the numerator of the exponent and combine terms we see that the exponent is bounded by

$$\frac{1}{4(t-\tau)} |s(t) - s(\tau)|(|x - s(t)| + |x - s(\tau)|) \le C_2(|x - s(t)| + |s(t) - s(\tau)|)$$

We have used the Lipschitz condition on the boundary to obtain the last inequality. Since we are going to let δ become close to zero and hence have τ become close to t and we want x to approach $s(t)$, we can assume that the last inequality is less than unity. This implies that the expression in the brackets in $J_1 - I_1$ will be bounded by

$$C_3(|x - s(t)| + |s(t) - s(\tau)|)$$

If we use this fact in $J_1 - I_1$ and use the known inequality $ye^{-y} \le C_4$ for $y \ge 0$, we will have

$$|J_1 - I_1| \le C_3 \int_{t-\delta}^{t} \frac{d\tau}{(t-\tau)^{1/2}} + C_3 \int_{t-\delta}^{t} d\tau \le C_{10} \delta^{1/2}$$

Since we know that $J_1 \to -\frac{1}{2}$ when $x \to s(t)$, that $|I_2| \leq C_5\delta^{1/2}$, and that $I = I_1+I_2$, we see that

$$\limsup_{x \to s(t)-0} \left| I + \frac{1}{2} \right| \leq C_6\delta^{1/2} \tag{B.1}$$

We can also see that $|I_1| \leq C_7$. We now define the integral K_0

$$K_0 \equiv \int_{t-\delta}^{t} \frac{|x - s(\tau)|}{2(t-\tau)} K(x,t;s(\tau),\tau)d\tau$$

We see that

$$K_0 \leq |I_1| + \int_{t-\delta}^{t} \frac{|s(t) - s(\tau)|}{2(t-\tau)} K(x,t;s(\tau),\tau)d\tau$$

The last integral is bounded because of the Lipschitz condition so we have

$$K_0 \leq C_8$$

We now introduce the integral K_1

$$K_1 \equiv \int_{t-\delta}^{t} \frac{|s(t) - s(\tau)|}{2(t-\tau)} K(s(t),t;s(\tau),\tau)d\tau$$

This integral is bounded by a constant because of the Lipschitz condition on the boundary $s(t)$. We now look at the equation

$$L = \int_0^t v(\tau)\frac{x - s(\tau)}{2(t-\tau)} K(x,t;s(\tau),\tau)d\tau - \int_0^t v(\tau)\frac{s(t) - s(\tau)}{2(t-\tau)} K(s(t),t;s(\tau),\tau)d\tau$$

We break L into the sum of two integrals $L = L_1 + L_2$ where

$$L_1 = \int_{t-\delta}^{t} v(\tau)\frac{x - s(\tau)}{2(t-\tau)} K(x,t;s(\tau),\tau)d\tau - \int_{t-\delta}^{t} v(\tau)\frac{s(t) - s(\tau)}{2(t-\tau)} K(s(t),t;s(\tau),\tau)d\tau$$

and

$$L_2 = \int_0^{t-\delta} v(\tau)\frac{x - s(\tau)}{2(t-\tau)} K(x,t;s(\tau),\tau)d\tau - \int_0^{t-\delta} v(\tau)\frac{s(t) - s(\tau)}{2(t-\tau)} K(s(t),t;s(\tau),\tau)d\tau$$

We see immediately that

$$\lim_{x \to s(t)} L_2 = 0$$

If we write $v(\tau) = v(t) + (v(\tau) - v(t))$ in our expression for L_1 and use (B.1) and the fact that K_0 and K_1 are bounded by constants, we see that

$$\limsup_{x \to s(t)-0} |L_1 + \frac{1}{2}v(t)| \leq C_9(\delta^{1/2} + \sup_{t-\delta \leq \tau \leq t} |v(t) - v(\tau)|$$

We thus have

$$\limsup_{x \to s(t)-0} |(L_1 + L_2) + \frac{1}{2}v(t)| \leq C_9(\delta^{1/2} + \sup_{t-\delta \leq \tau \leq t} |v(t) - v(\tau)|$$

Since the left side is independent of δ and the right side goes to zero when $\delta \to 0$, we have

$$\limsup_{x \to s(t)-0} |(L_1 + L_2) + \frac{1}{2}v(t)| = 0$$

This is equivalent to

$$\lim_{x \to s(t)-0} \frac{\partial}{\partial x} \int_0^t v(\tau)K(x, t; s(\tau), \tau)d\tau = \frac{1}{2}v(t) + \int_0^t v(\tau) \left[\frac{\partial}{\partial x}K(x, t; s(\tau), \tau)\right]_{x=s(t)} d\tau$$

This completes our derivation. We have followed closely the proof given in (7:217–219).

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Vita

Captain Donald C. Vosika was born on 24 March 1952 in Edgewater, Florida. In 1969 he graduated from Maynard High School, Maynard, Minnesota. He graduated from Moorhead State University, Moorhead, Minnesota with a Bachelor of Science degree in Mathematics and Physics in 1973. Captain Vosika joined the Air Force in 1982 and received his commission from the Officer Training School in San Antonio, Texas. He received his Bachelor of Science degree in Electrical Engineering from the Air Force Institute of Technology in 1985. Captain Vosika was then assigned to the Avionics Laboratory at Wright-Patterson AFB as a computer networks systems engineer. He entered the School of Engineering, Air Force Institute of Technology, in May 1988.

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